# San Jacinto River: Modeling Workshop #2
## Preliminary Model Calibration Results

**Presented by**
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**November 10, 2011**

# Meeting Agenda

| | |
|---|---|
| Introductions/review of modeling objectives | 8:00 - 8:15 |
| Review of modeling framework | 8:15 – 8:30 |
| Hydrodynamic model calibration | 8:30 – 9:30 |
| • *Review of ADCP data collected during 2010 and 2011* | |
| • *Calibration approach* | |
| • *Calibration results* | |
| BREAK | 9:30 – 9:45 |
| Sediment transport model calibration | 9:45 – 10:45 |
| • *Geochronology analysis of radioisotope cores* | |
| • *Calibration approach* | |
| • *Calibration results* | |
| Chemical fate and transport model | 10:45 – 11:45 |
| • *Review of key model inputs and underlying datasets* | |
| • *Model development updates* | |
| • *Calibration approach* | |

# Presentation Overview

- Review of modeling objectives
- Review of modeling framework
- Hydrodynamic model
- Sediment transport model
- Chemical fate and transport model

# Review of Modeling Objectives

# Primary Objectives

- Develop CSMs for sediment transport and chemical fate and transport
- Develop and apply models that can be used as a management tool to evaluate the effectiveness of various remedial alternatives
- Answer specific questions about sediment transport and chemical fate and transport processes within the Study Area

# Questions: Sediment Transport Model

- What areas are net depositional, net erosional, or in dynamic equilibrium?
- What is the net sedimentation rate in areas that are net depositional?
- What is the potential scour depth during high-flow events or storms?
- What is the fate of sediment eroded from the waste impoundment area?

# Questions:
## Chemical Fate and Transport Model

- What is the fate of particle-associated chemicals that are remobilized from the waste impoundment area under current conditions?
- What is the rate of natural attenuation of chemical concentrations in surface-layer sediment in locations that may be impacted by releases from the waste impoundment?

# Questions:
# Chemical Fate and Transport Model (cont.)

- What are the effects of high-flow events or storms on chemical concentrations in the surface layer of the sediment bed and in the water column?
- What is the potential for erosion, transport, and re-deposition of particle-associated chemicals buried below the surface layer of the bed during high-flow events or storms?



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# Review of Modeling Framework

# SJR Modeling Framework

**Hydrodynamic Model:**
**EFDC**
Current velocity
Stage height/water depth
Bed shear stress

↓

**Sediment Transport Model:**
**SEDZLJ**
Total suspended solids (TSS) concentration
Bed elevation change
Erosion/deposition zones
Net sedimentation rate

↓

**Chemical Fate and Transport Model:**
**QEA-FATE**
Water column chemical concentration
Bed chemical concentration



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# SJR Modeling Framework:
## Previous Modeling Studies

- Models have been applied to a wide range of sites
  - Patrick Bayou (TX)
  - Upper Hudson River (NY)
  - Lower Duwamish Waterway (WA)
  - Lower Willamette River (OR)
- Models have undergone peer review as well as project-specific agency reviews



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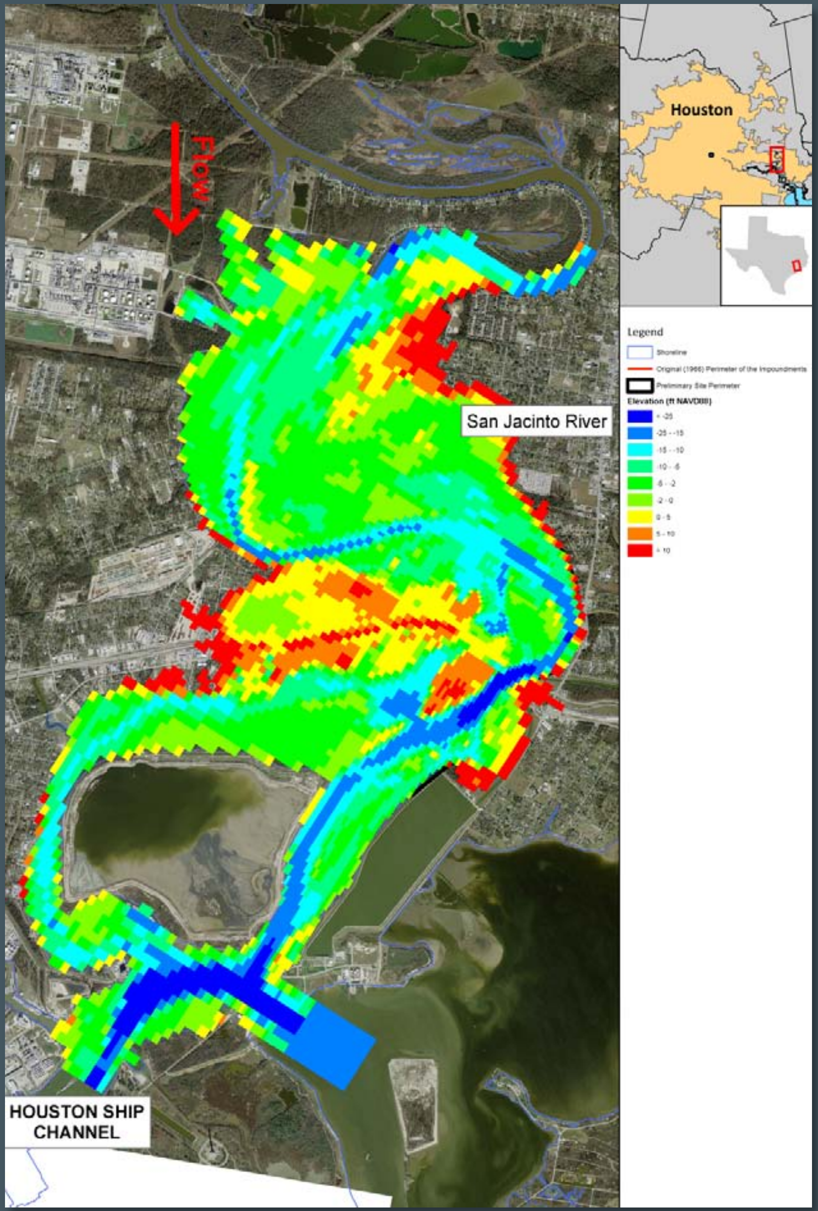
# Hydrodynamic Model

# Numerical Grid

- Approximately 6,400 grid cells
- Includes HSC and SJR channel up to dam
- 100-foot resolution within site perimeter
- Simulation times
  - Hydro: 66 hours/year
  - Sedtran: 6 hours/year



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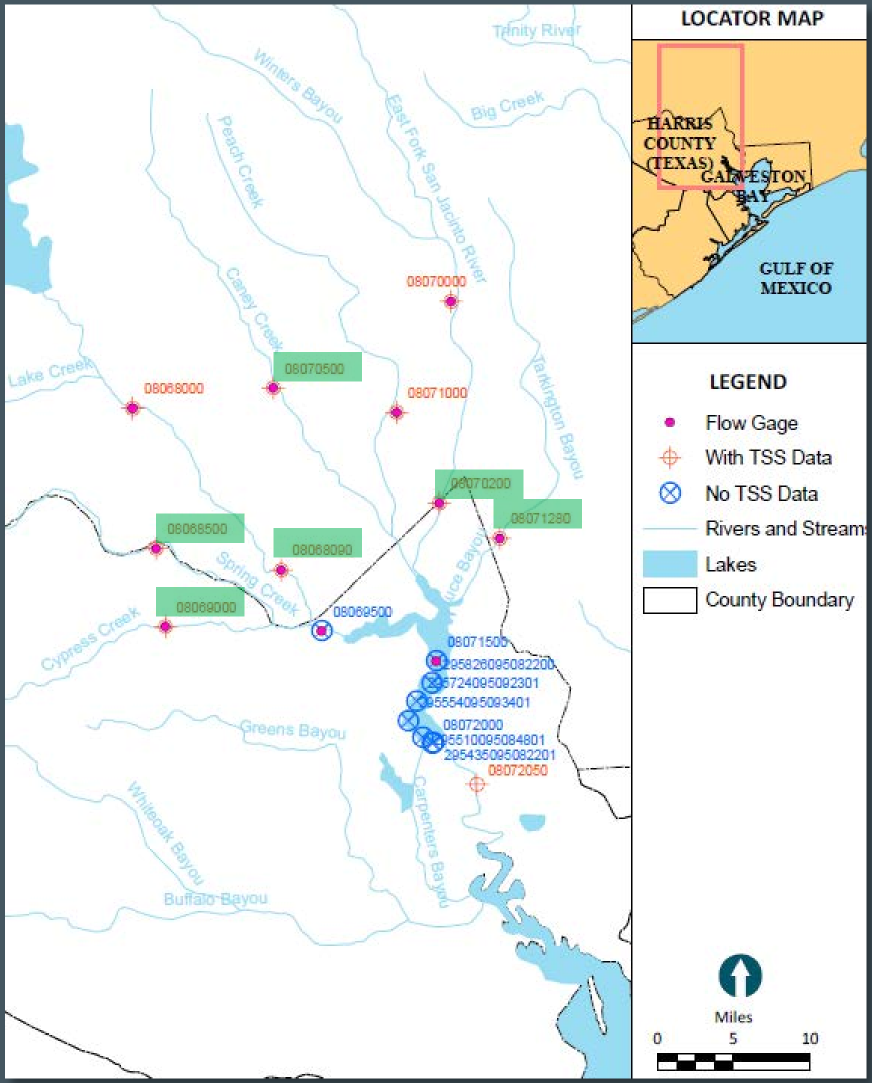
# Boundary Condition:
## Flow Rate at Lake Houston Dam

- June 2005 to present
  - CWA flow rate data
- July 1996 to June 2005
  - U.S. Geological Survey (USGS) stage height data (correlation between stage height and flow rate)

# Boundary Condition: Flow Rate at Lake Houston Dam

- Before July 1996
  - Estimated using flow rate data collected at six USGS gauging stations located upstream of Lake Houston



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# Boundary Condition: Flow Rate Into HSC

- Inflow to the HSC was estimated using USGS data collected on five sub-basins
  - Buffalo Bayou
  - Sims Bayou
  - Vince Bayou
  - Hunting Bayou
  - Greens Bayou



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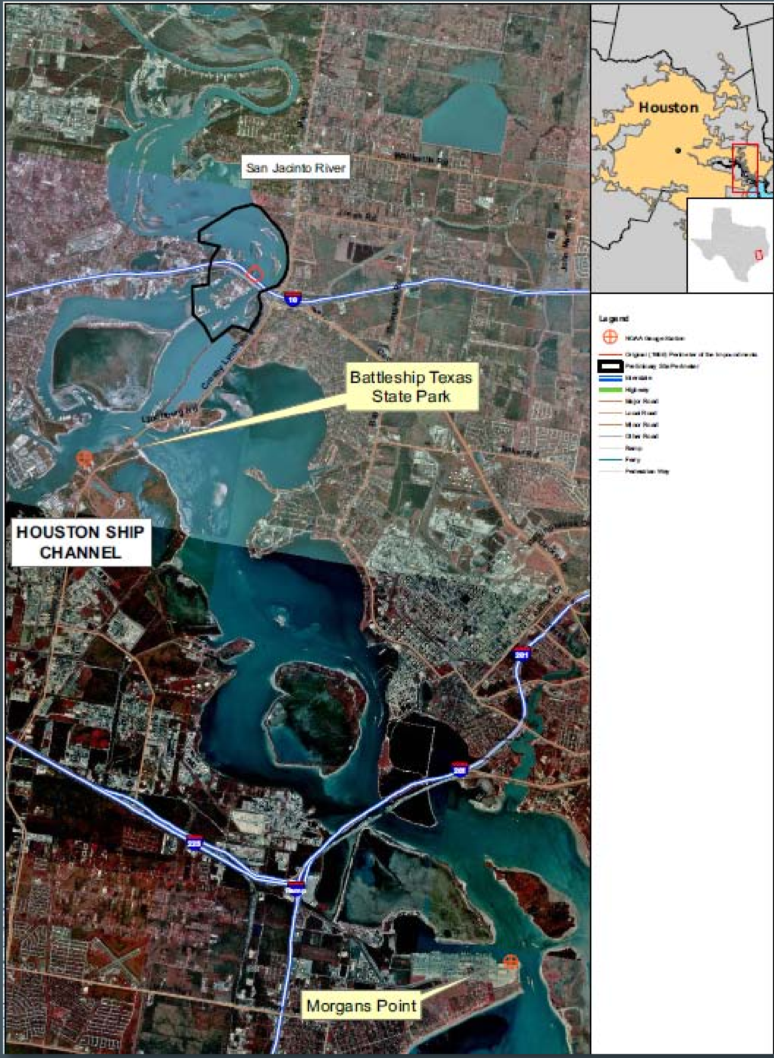
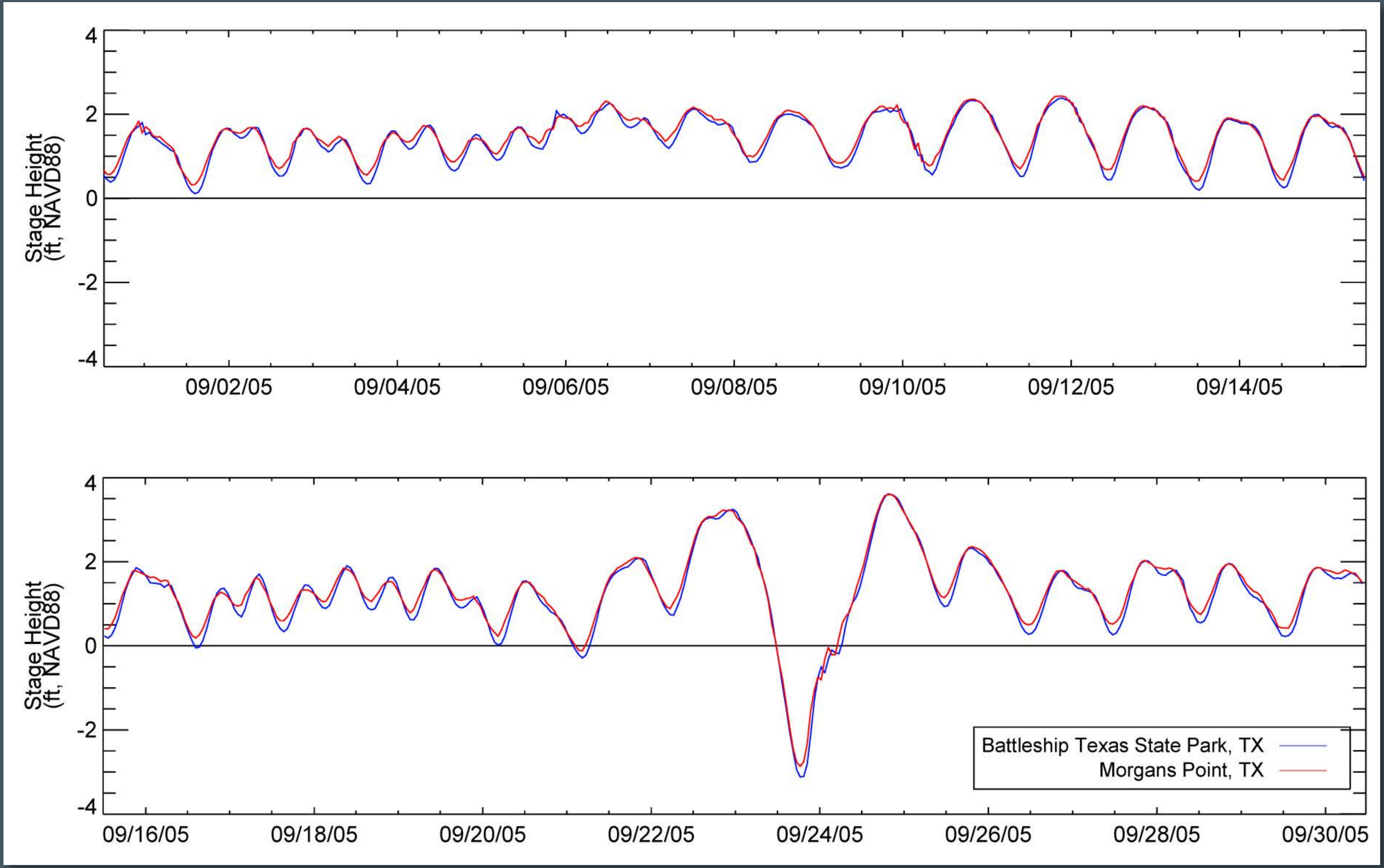
# Boundary Condition: Tidal Elevation

- Specified using hourly data collected at National Oceanic and Atmospheric Association (NOAA) gauging station located at Morgan's Point
- Strong correlation exists between tidal elevations at Morgan's Point and Battleship Texas



# Boundary Condition:
## Tidal Elevation (cont.)



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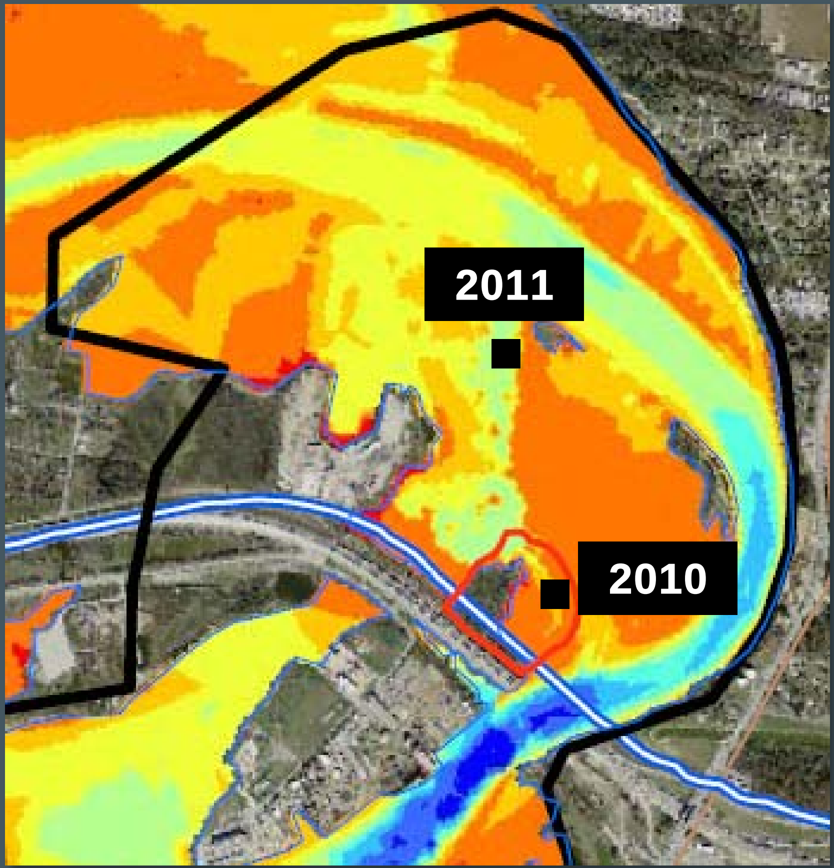
# Hydrodynamic Model: Calibration Strategy

- Use current velocity and stage height data collected during 2010 and 2011
- Adjustable parameter: effective bed roughness
- Calibration value: 1 cm



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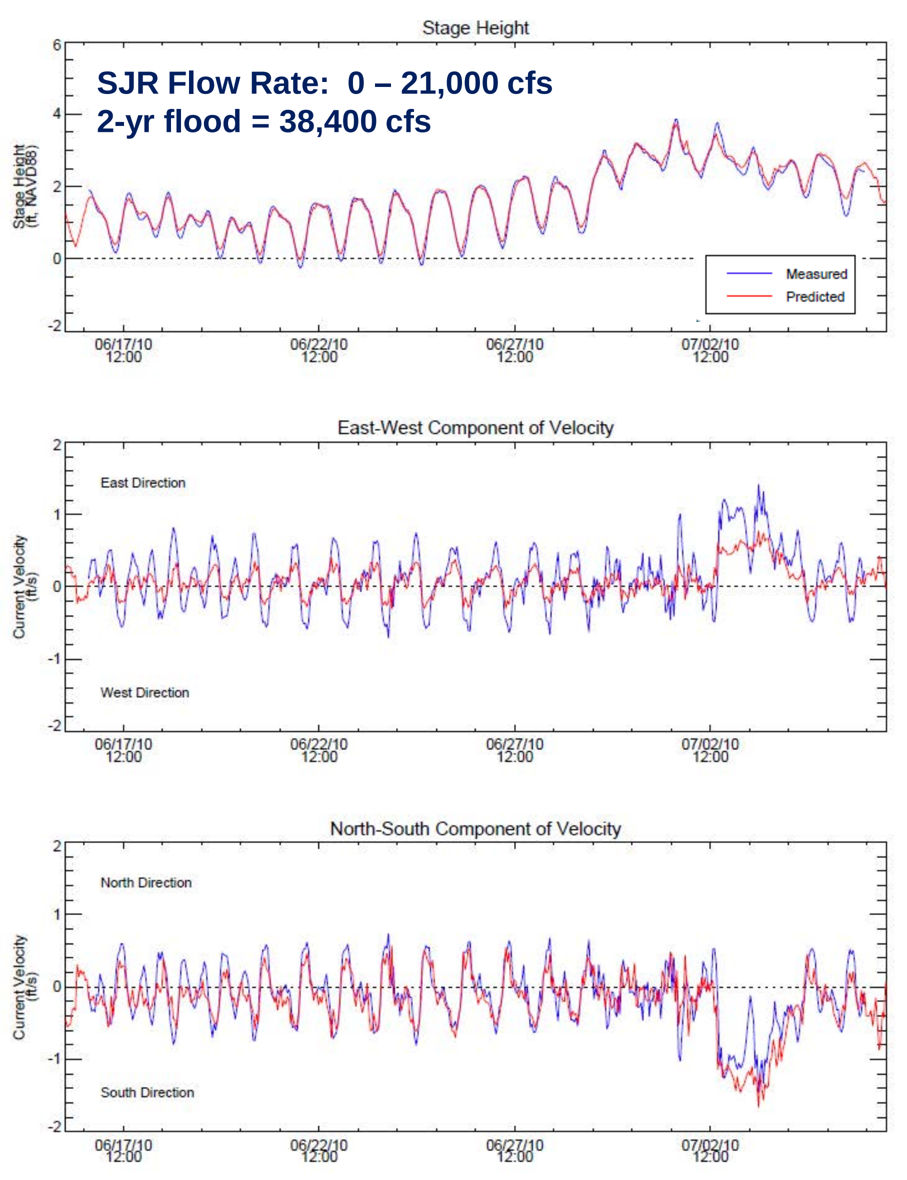
# Calibration Results: June to July 2010



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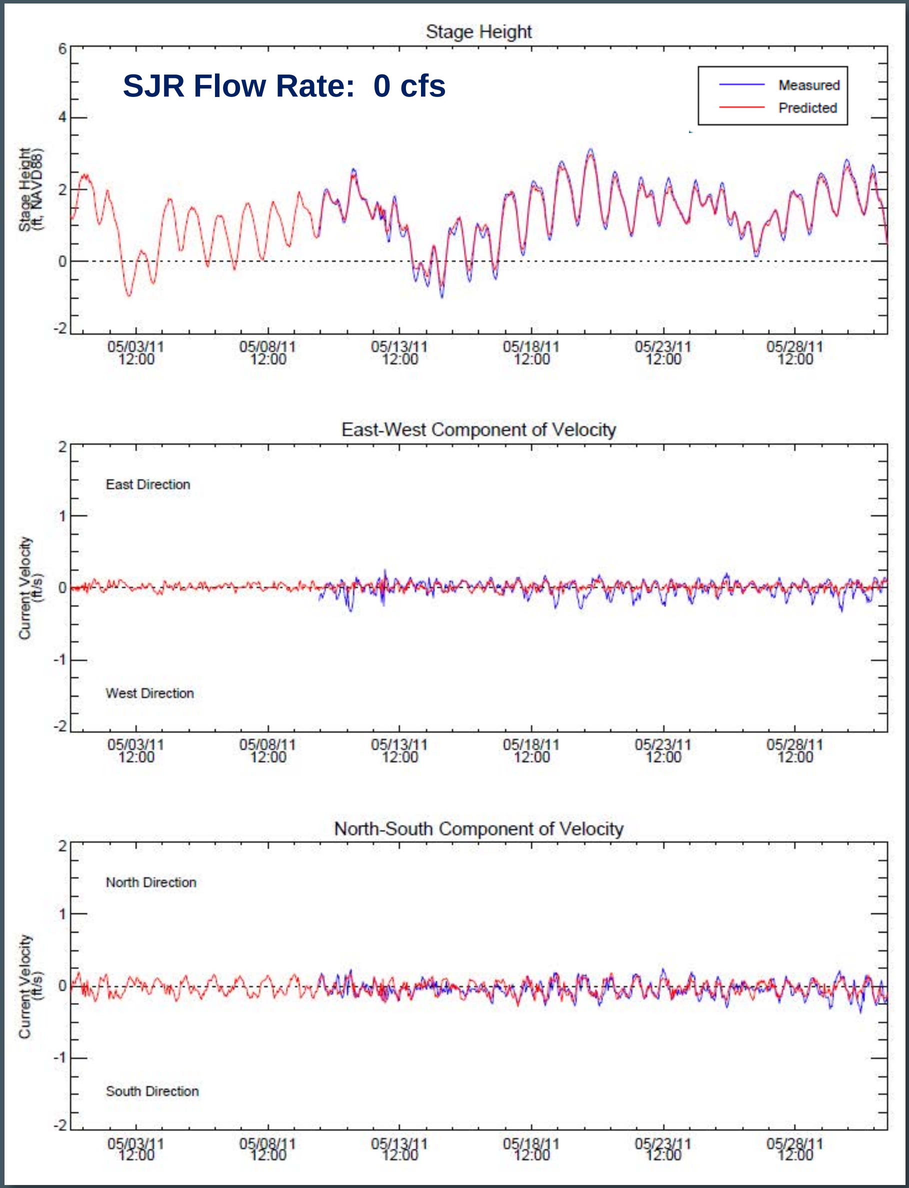
# Calibration Results:
# May 2011



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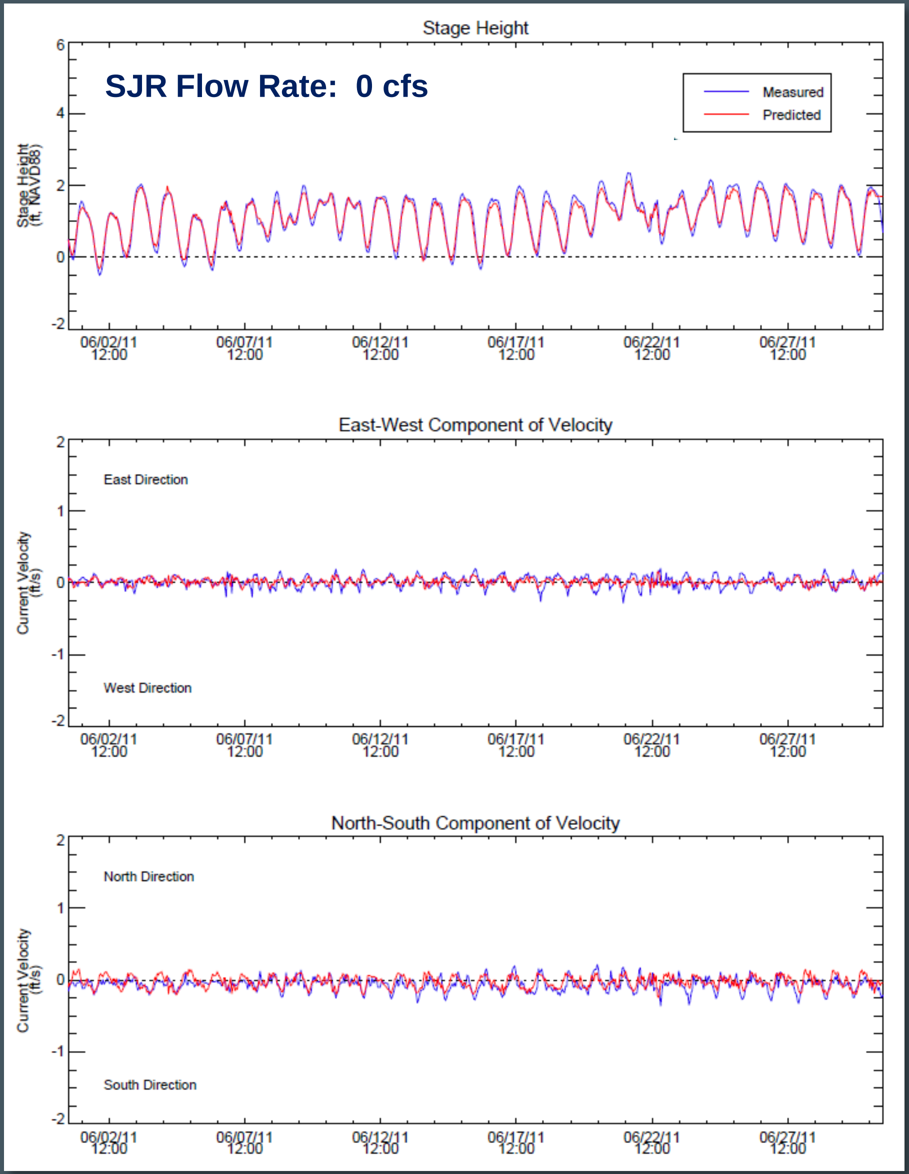
# Calibration Results: June 2011



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# BREAK (?)

# Sediment Transport Model

# Sediment Size Classes and Settling Speeds

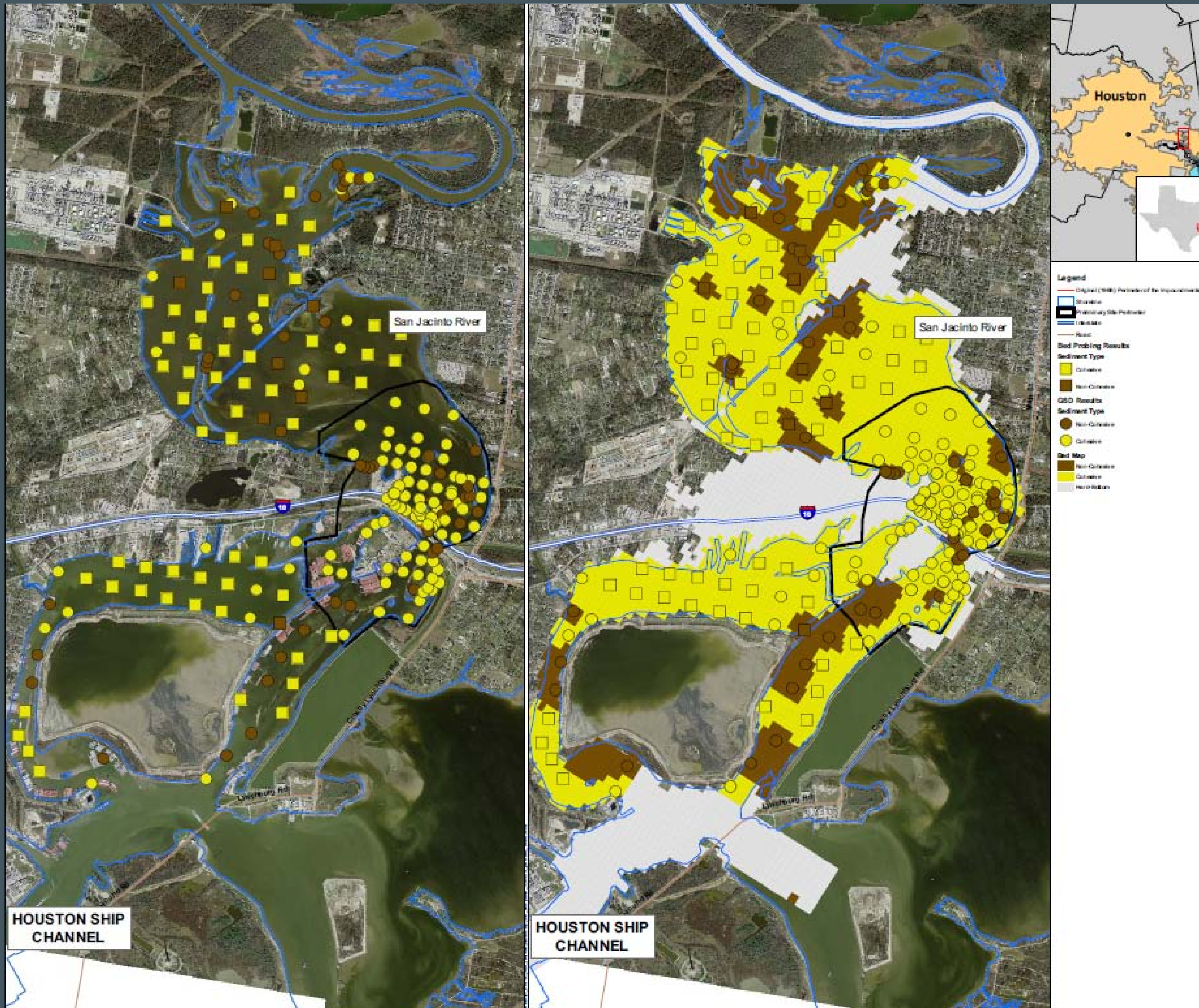
- Effective particle diameters were estimated for classes 2,3, and 4 using GSD data from 168 samples (0-1 ft) collected during 2010 and 2011

| Sediment Size Class | Effective Particle Diameter (µm) | Settling Speed (m/day) |
| --- | --- | --- |
| 1: clay/silt | N/A | Calibration parameter |
| 2: fine sand | 140 | 870 |
| 3: medium/coarse sand | 510 | 5,200 |
| 4: gravel | 3,500 | 21,700 |

# Specification of Sediment Transport Model Inputs

- The following model inputs were specified using site-specific data
  - Sediment bed map
  - Bulk bed properties
    - Median particle diameter ($D_{50}$), effective bed roughness ($D_{90}$) initial bed composition, bulk (dry) density
  - Erosion rates of cohesive sediment
  - Incoming sediment load

# Sediment Bed Map



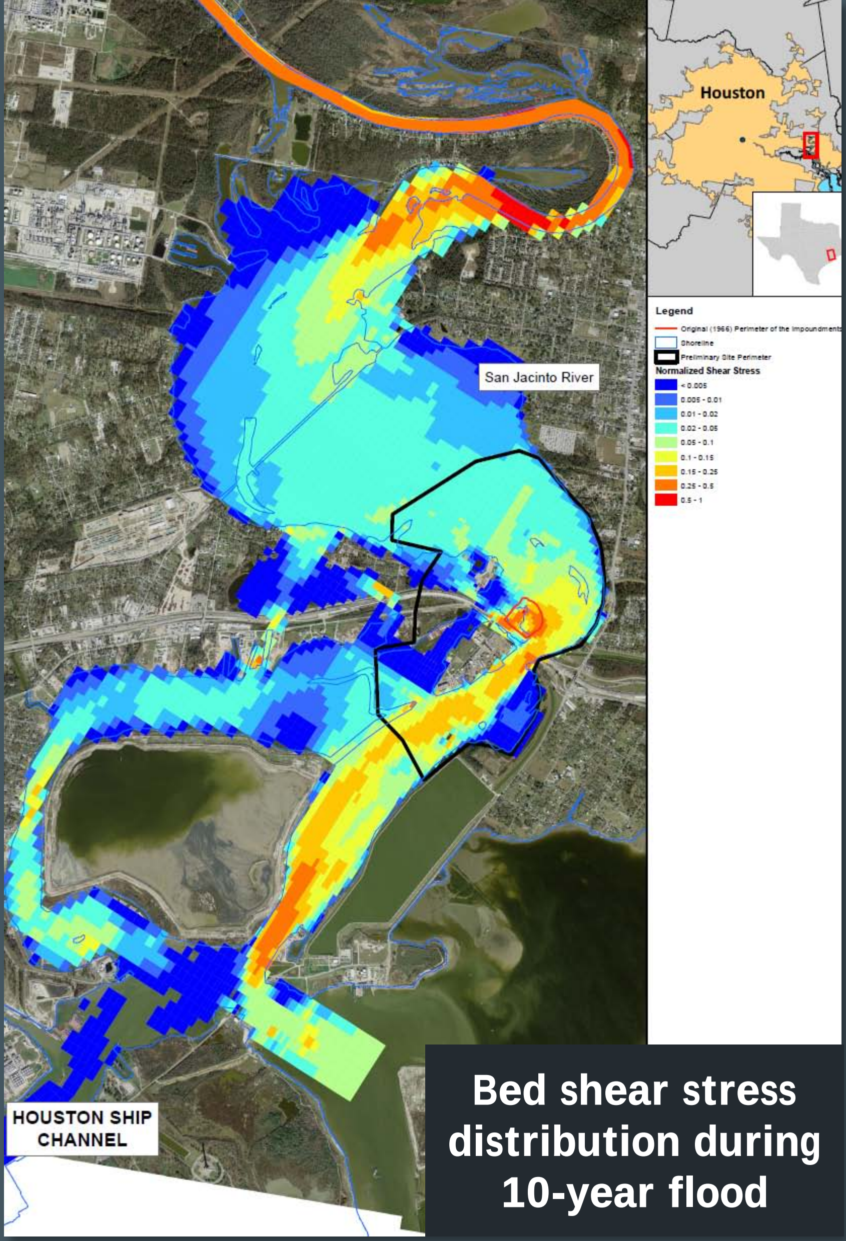
# Sediment Bed Properties: Initial Composition

- Based on GSD data from 168 samples (0-1 ft) collected during 2010 and 2011
- Developed method to generate spatial distribution of $D_{50}$ and bed composition

| Sediment Class | Average Content: Cohesive Bed (%) | Average Content: Non-Cohesive Bed (%) |
|---|---|---|
| 1: clay/silt | 51 | 11 |
| 2: fine sand | 32 | 36 |
| 3: coarse sand | 12 | 47 |
| 4: gravel | 5 | 6 |

# Spatial Distribution: $D_{50}$

- Assumed that there is a functional relationship between $D_{50}$ and bed shear stress
- Higher $D_{50}$ in areas of higher bed shear stress
- Have used similar approach in other studies




**Bed shear stress distribution during 10-year flood**



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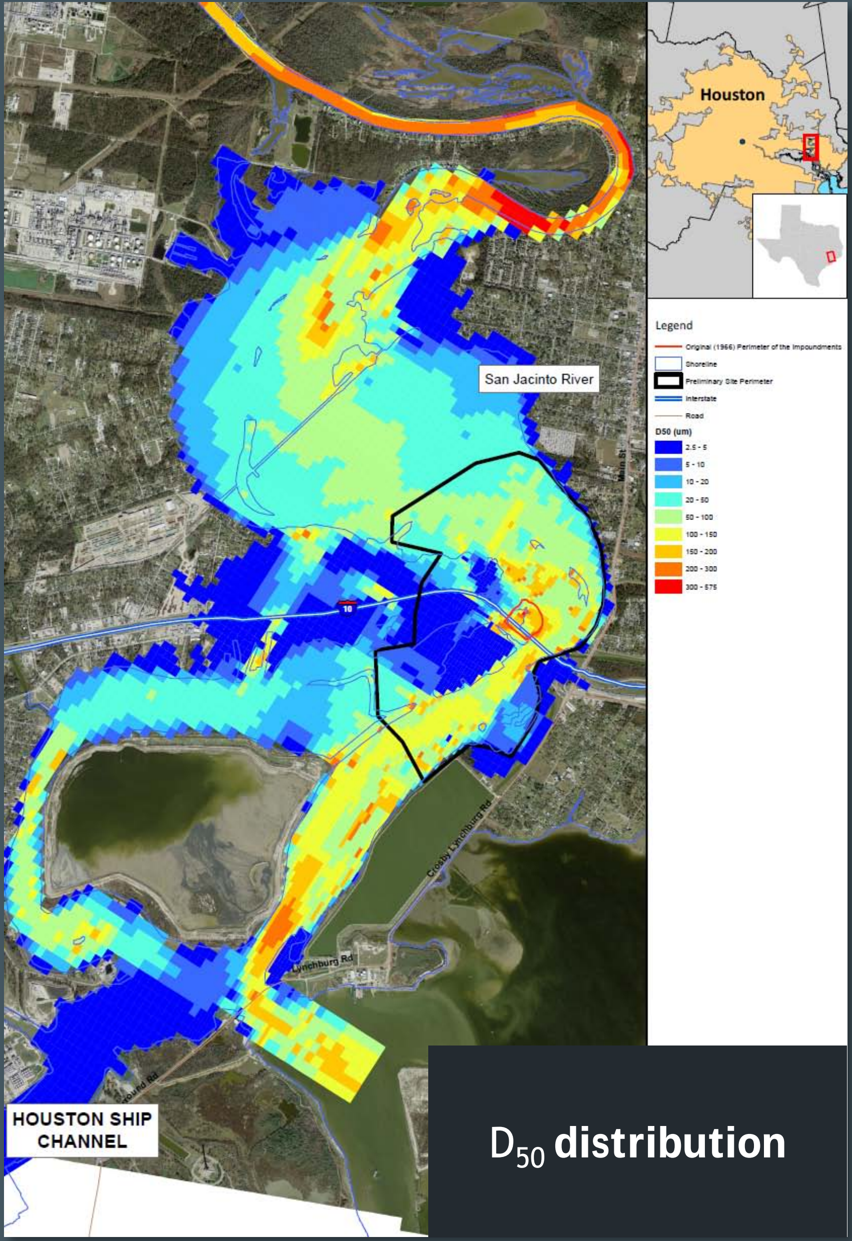
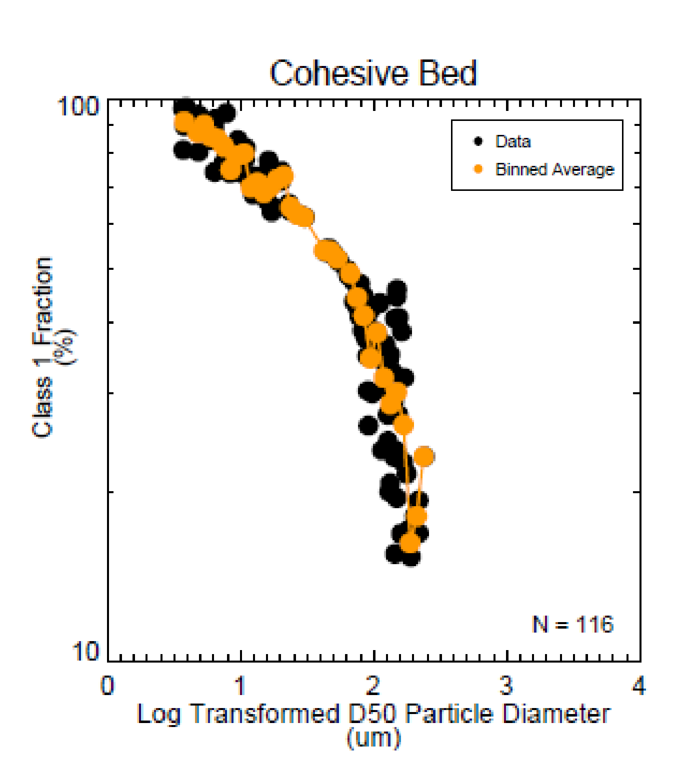
# Spatial Distribution: $D_{50}$ (cont.)

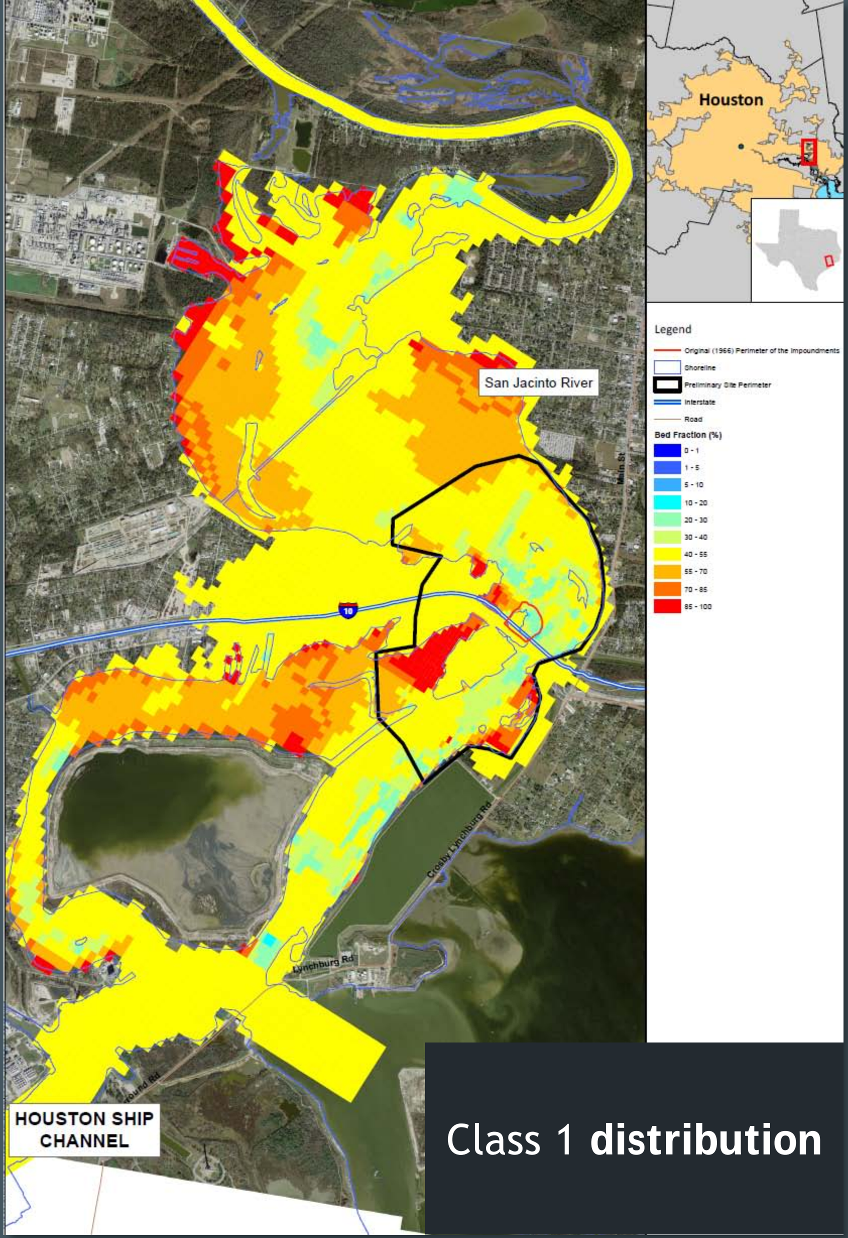
- Used GSD data to constrain $D_{50} = f(\tau)$
- Next step was to develop correlations between $D_{50}$ and bed composition using GSD data




$D_{50}$ distribution

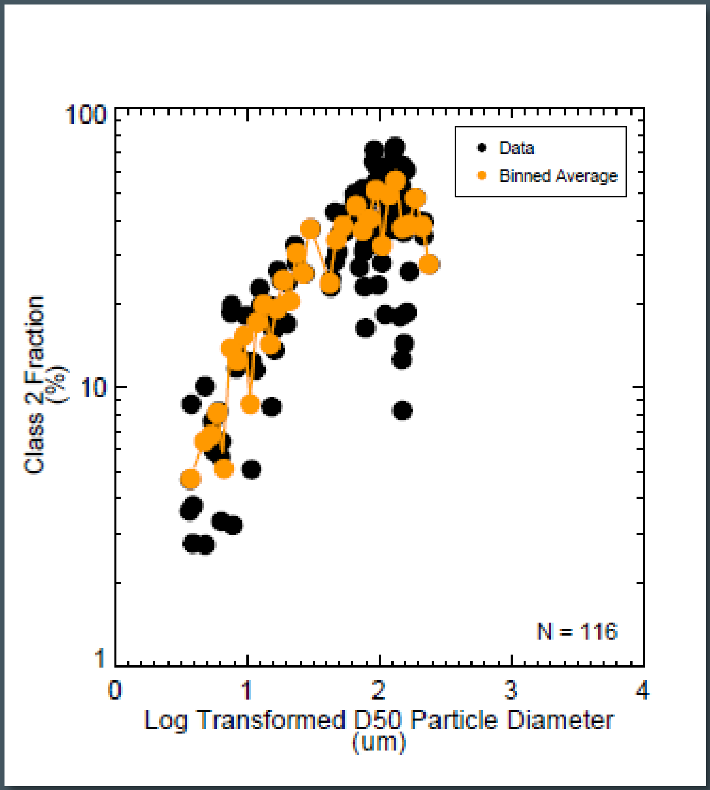
# Initial Composition: Clay/Silt

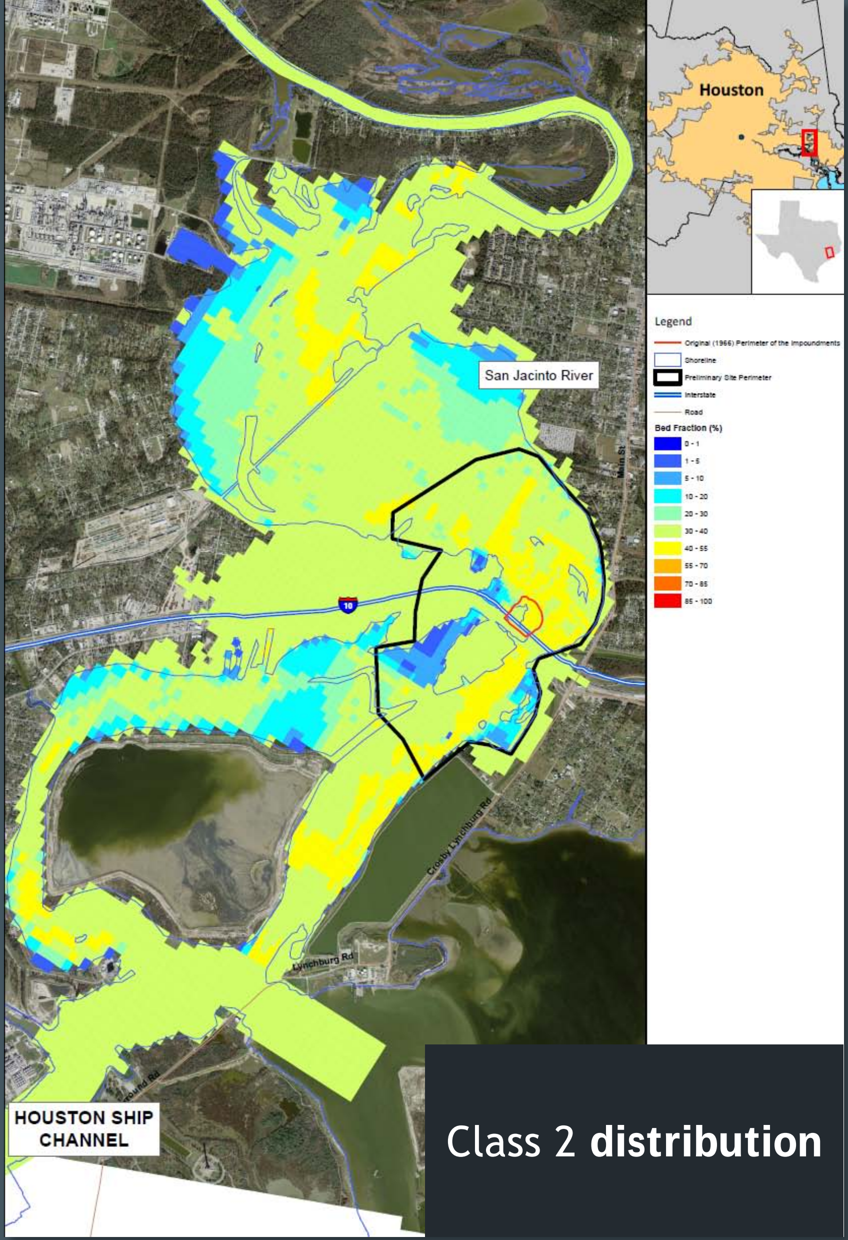



Class 1 **distribution**

# Initial Composition: Fine Sand




Class 2 **distribution**



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# Sediment Transport Model: Calibration Strategy

- Primary calibration target is net sedimentation rates (NSR) determined from radioisotope core data collected at ten locations during May 2011
- TSS concentration data received from TCEQ will be used to the fullest extent possible to evaluate model performance



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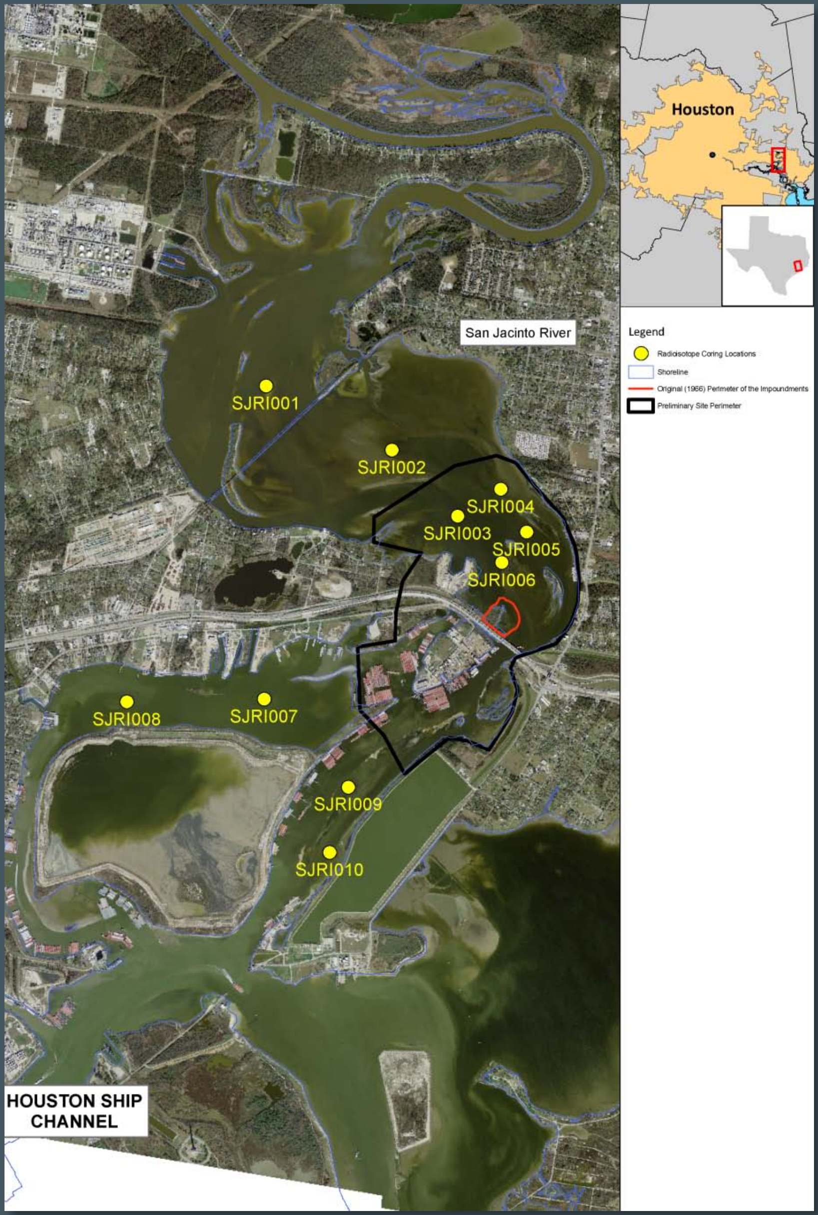
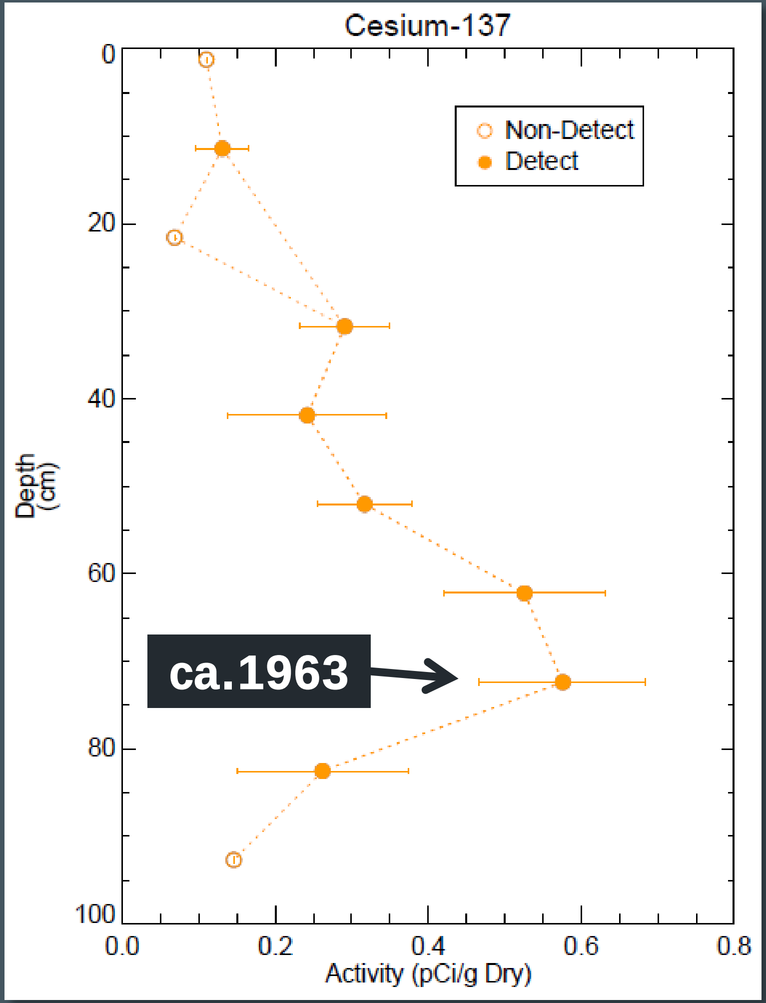
# Radioisotope Coring Study



# Geochronology Analysis:
## Age-Dating Using Cs-137 Data

- Peak Cs-137 activity corresponds to circa 1963
- Provides average NSR during 48-year period (1963 to 2011)



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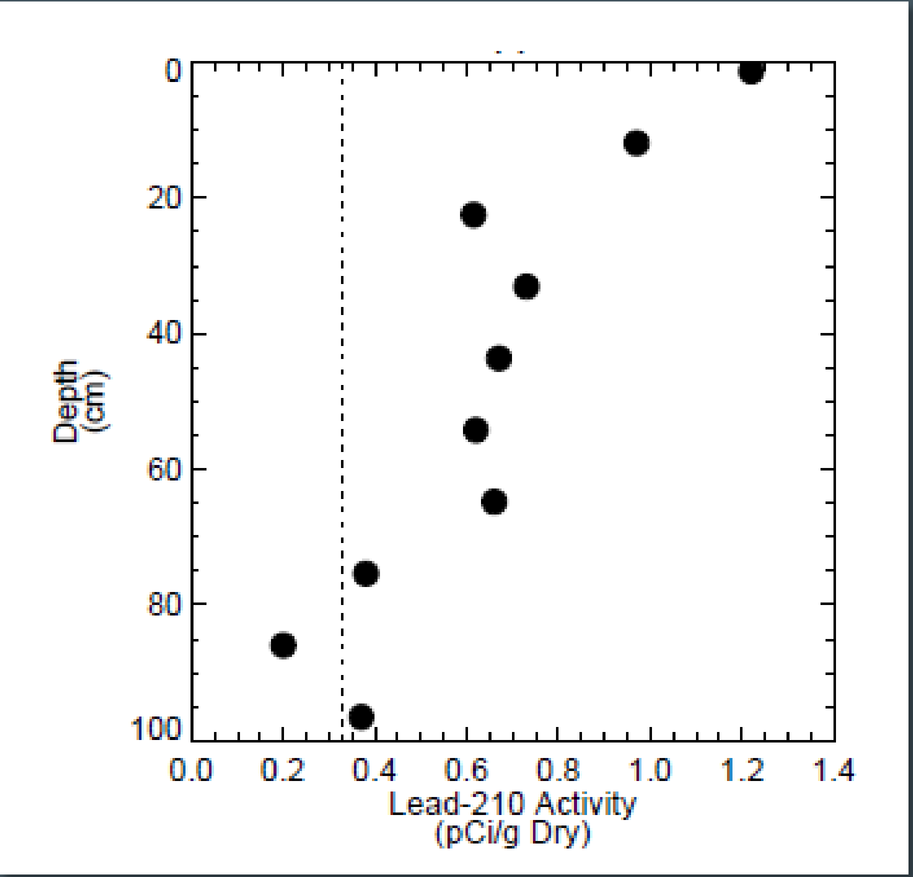
# Geochronology Analysis:
## Age-Dating Using Pb-210 Data

- NSR is determined from rate of decreasing Pb-210 activity with increasing depth



# Geochronology Analysis

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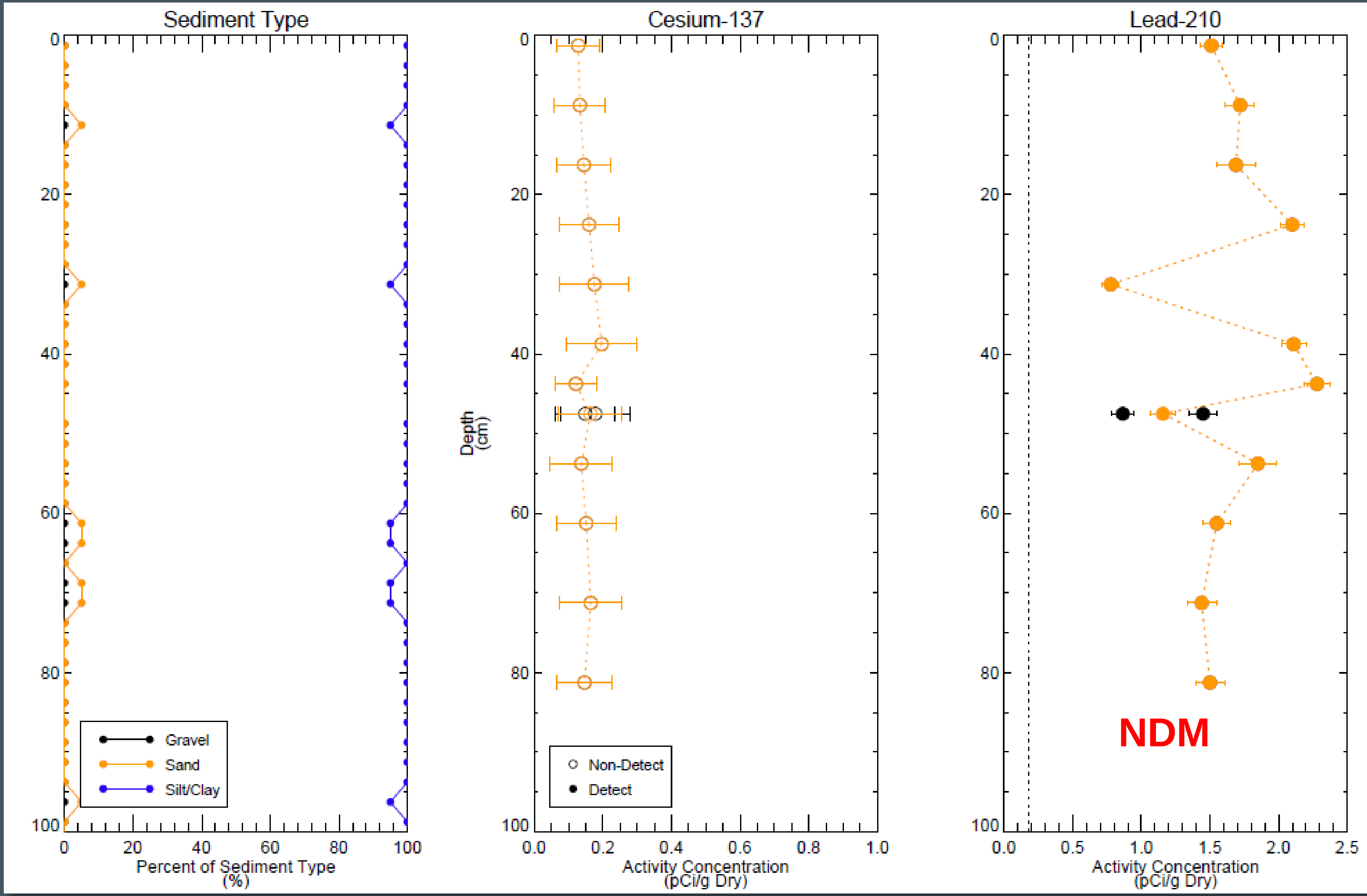
# Geochronology : Core 3



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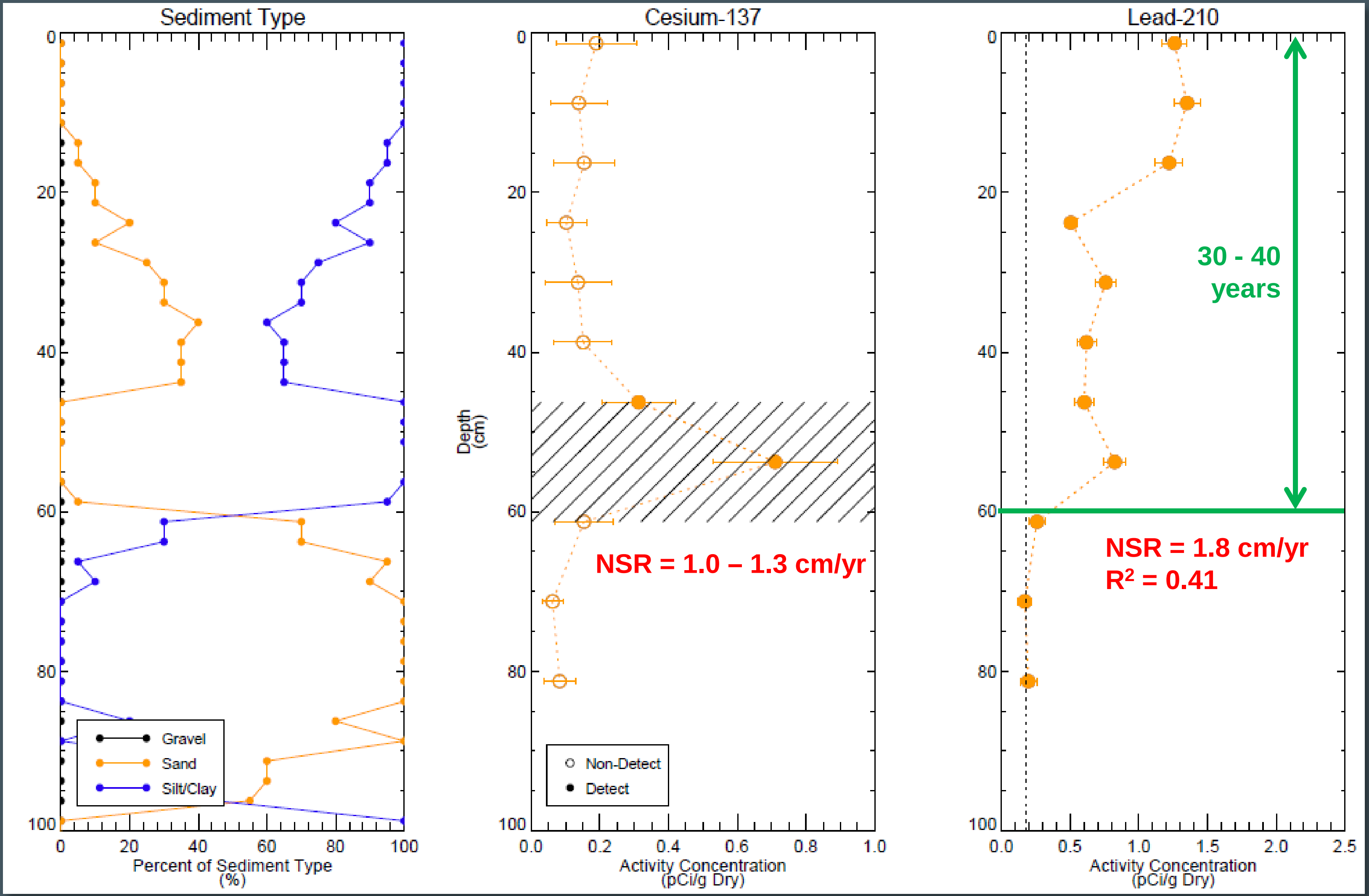
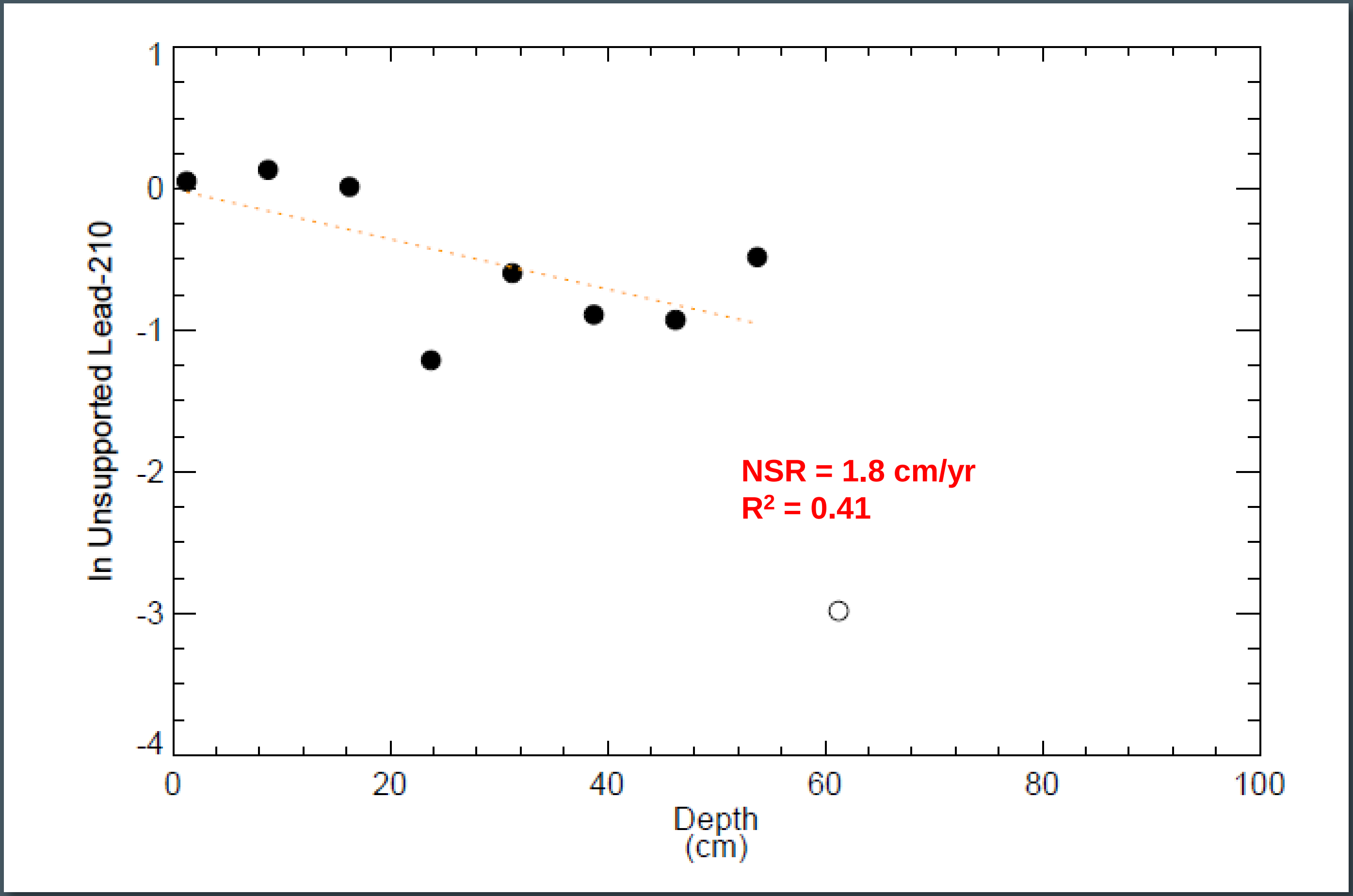
# Geochronology : Core 5 – Method 1



# Geochronology : Core 5 – Method 1 (cont.)



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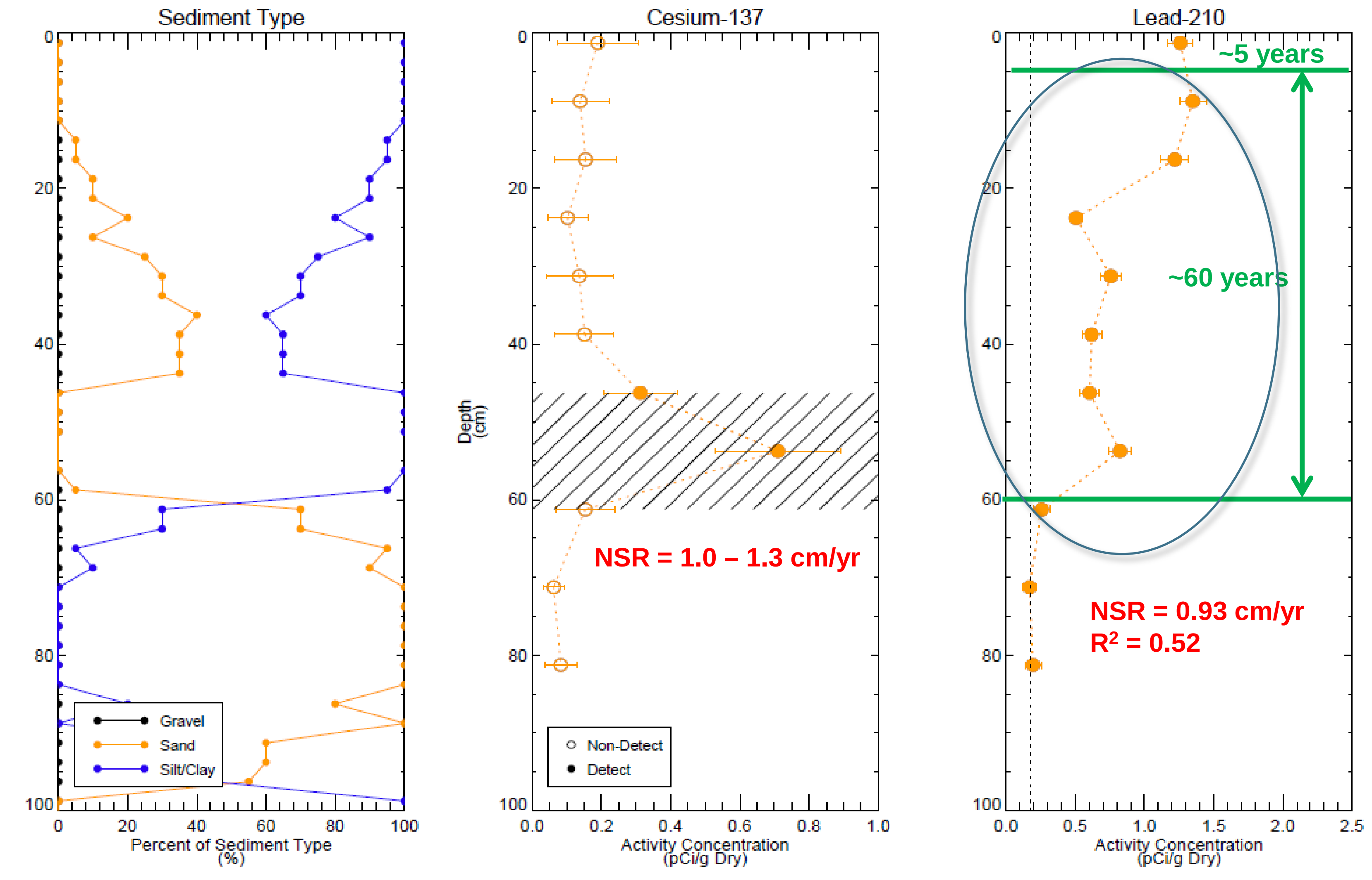
# Geochronology : Core 5 – Method 2



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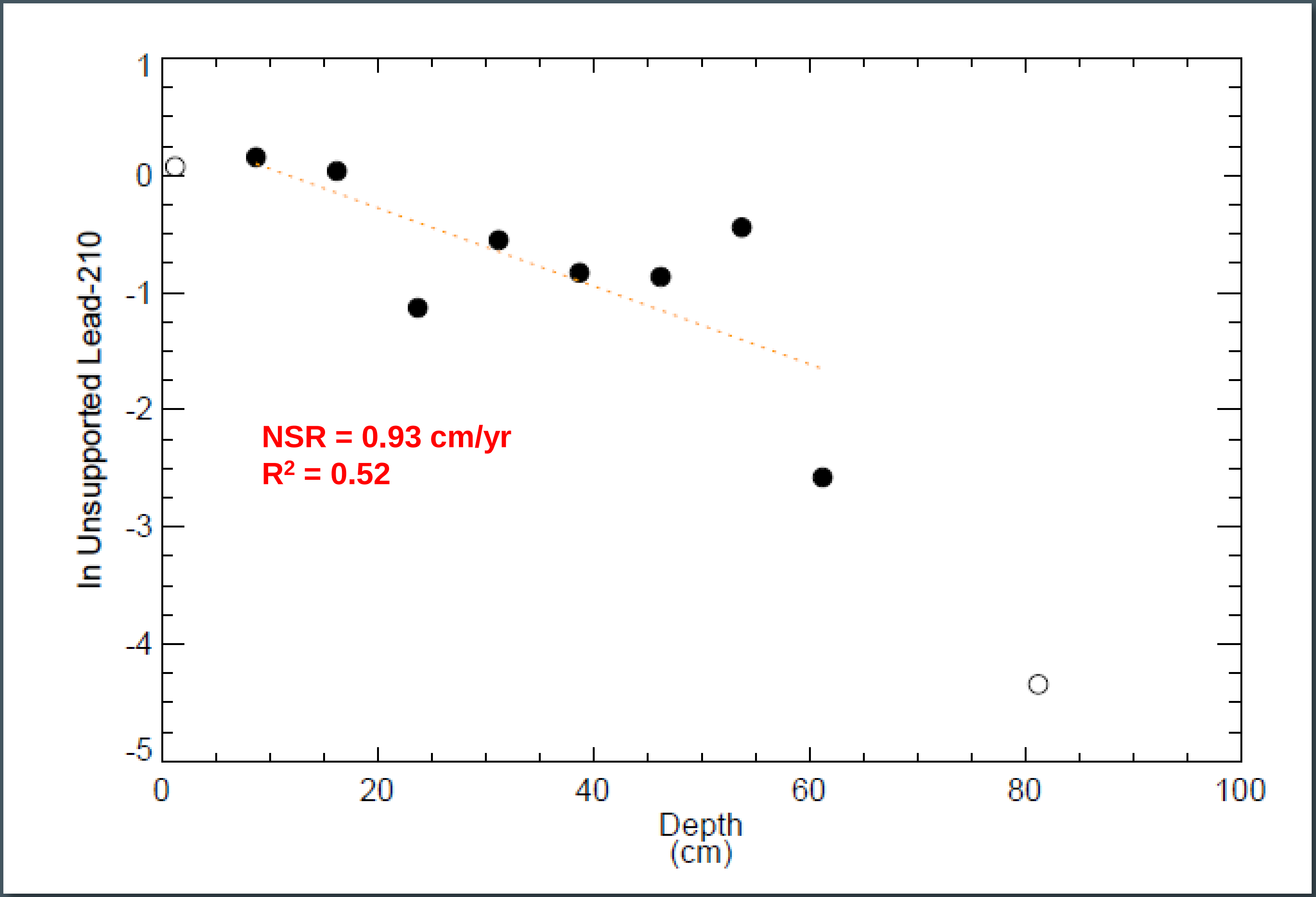
# Geochronology : Core 5 – Method 2 (cont.)



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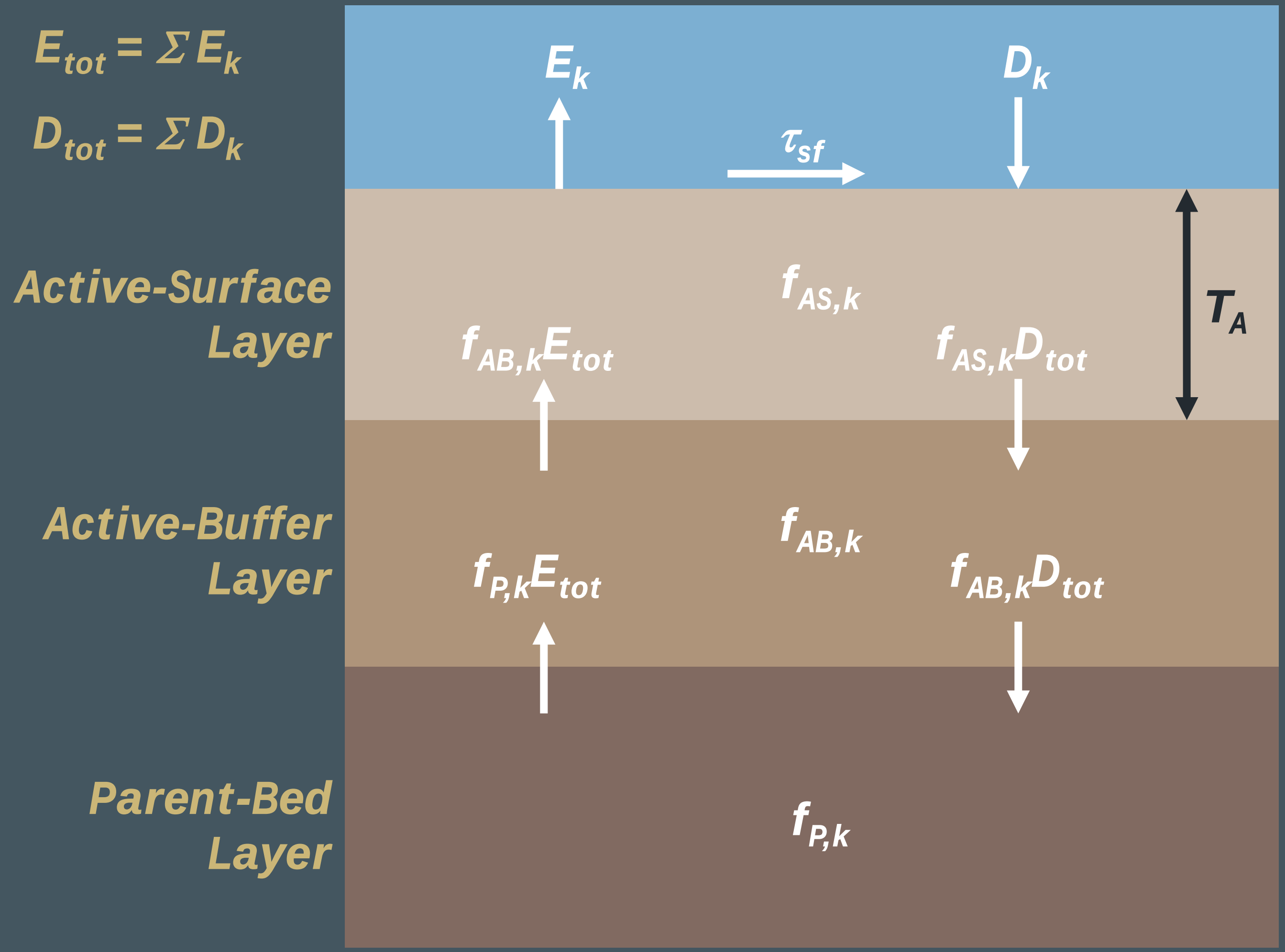
# Sediment Transport Model:
## Calibration Strategy

- 21-year (1990 to 2010) simulation was conducted
- Predicted NSR values were compared to estimated NSR values
- Model parameters may be adjusted during calibration
  - Settling speed of class 1 (clay/silt)
    - Typical range: approximately 1 to 20 meters/day
- Active layer thickness in cohesive bed

# Cohesive Bed Erosion: Bed Model

$E_{tot} = \Sigma E_k$

$D_{tot} = \Sigma D_k$




$= 2\ d_m\ (\tau_{sf}/\tau_{cr})^n$

$d_m$ = mean diameter

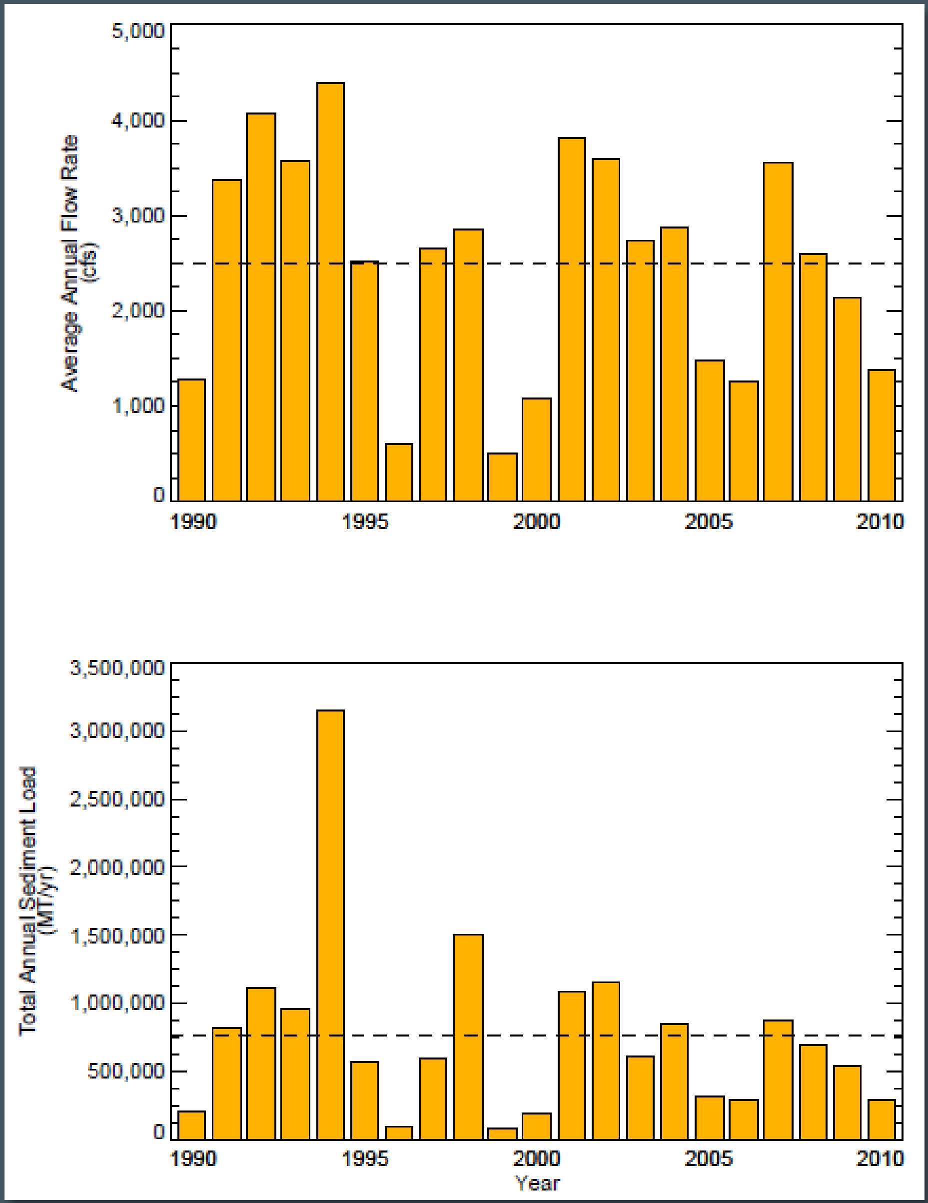
$\tau_{sf}$ = skin friction shear stress

$\tau_{cr}$ = critical shear stress

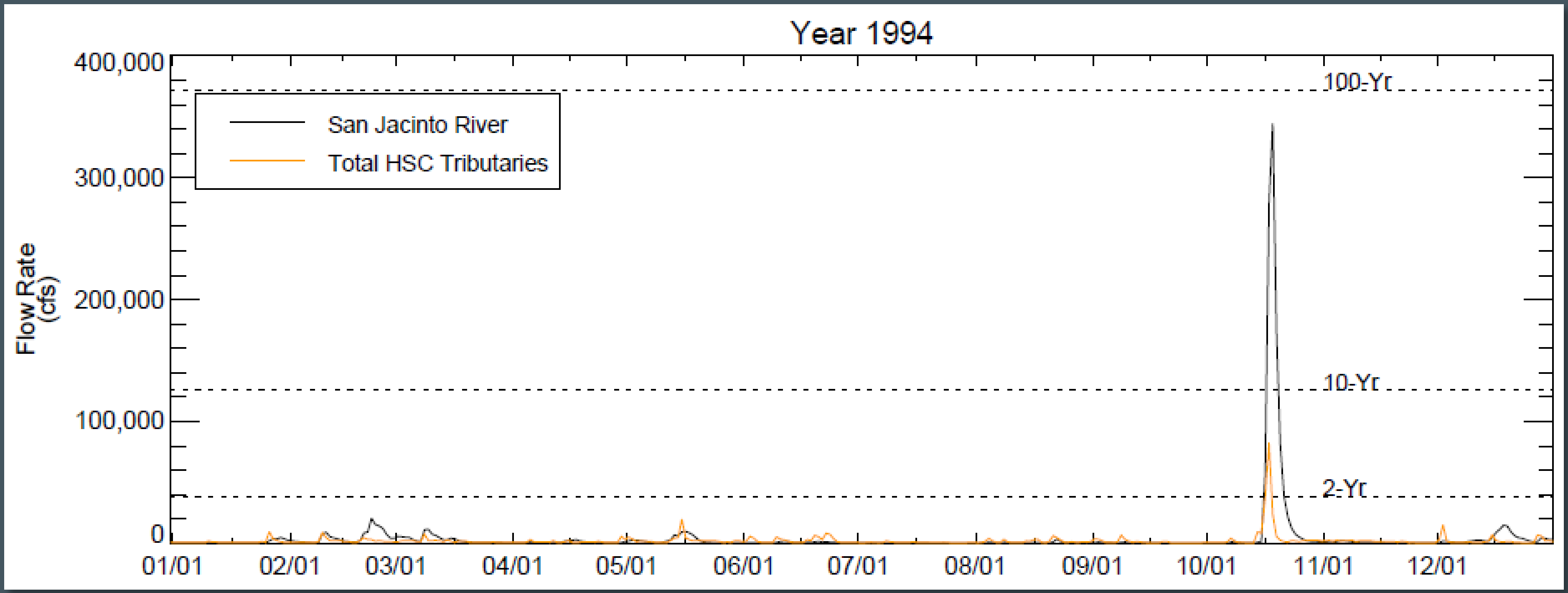
$n$ = adjustable exponent (0.1 -1)

Schematic of interactions between the water column, active layer, and parent-bed layer when the active-buffer layer is present

# 21-Year Calibration Period: 1990 to 2010



# 21-Year Calibration Period: 1990 to 2010



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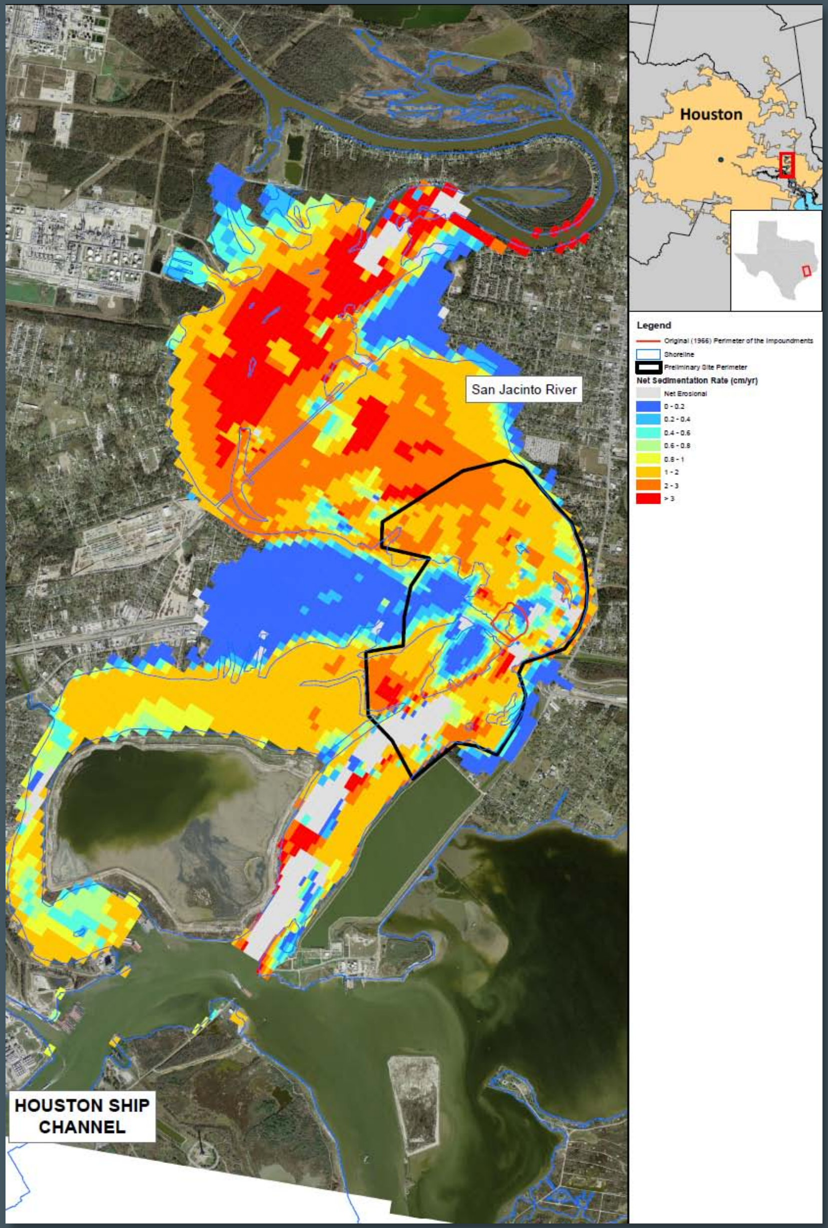
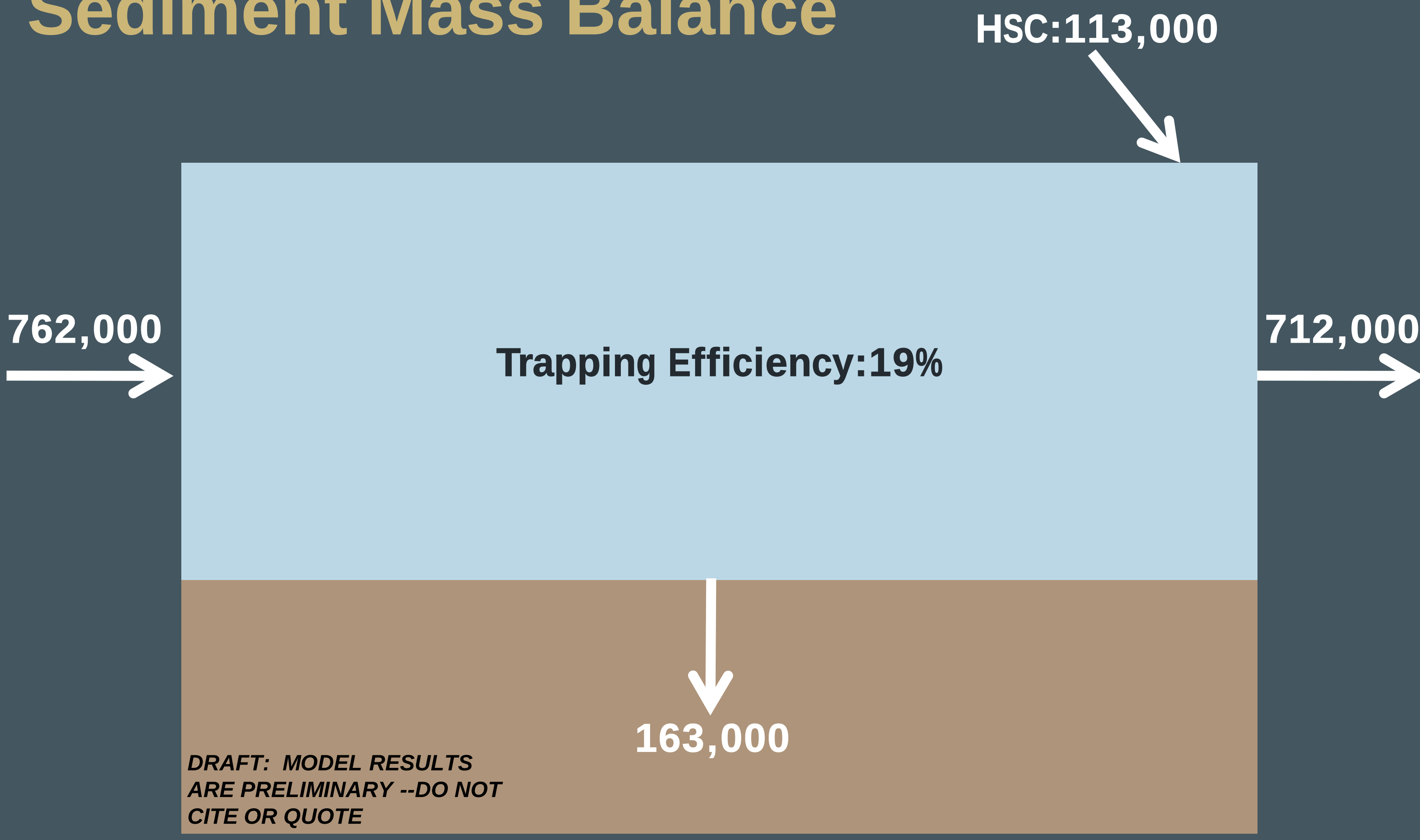
# Preliminary Calibration Results: Average NSR




***DRAFT: MODEL RESULTS ARE PRELIMINARY***
***-- DO NOT CITE OR QUOTE***

# 21-Year Calibration Period:
## Sediment Mass Balance




**Units: metric tons/year**

# Chemical Fate and Transport Model

# Outline – Fate Model

- Review model structure and processes
- Model development
  - Review of key model inputs and underlying datasets
  - Model input updates
    - Expansion to include OCDD
    - Specification of external loads
    - Development of organic carbon inputs
- Model calibration approach



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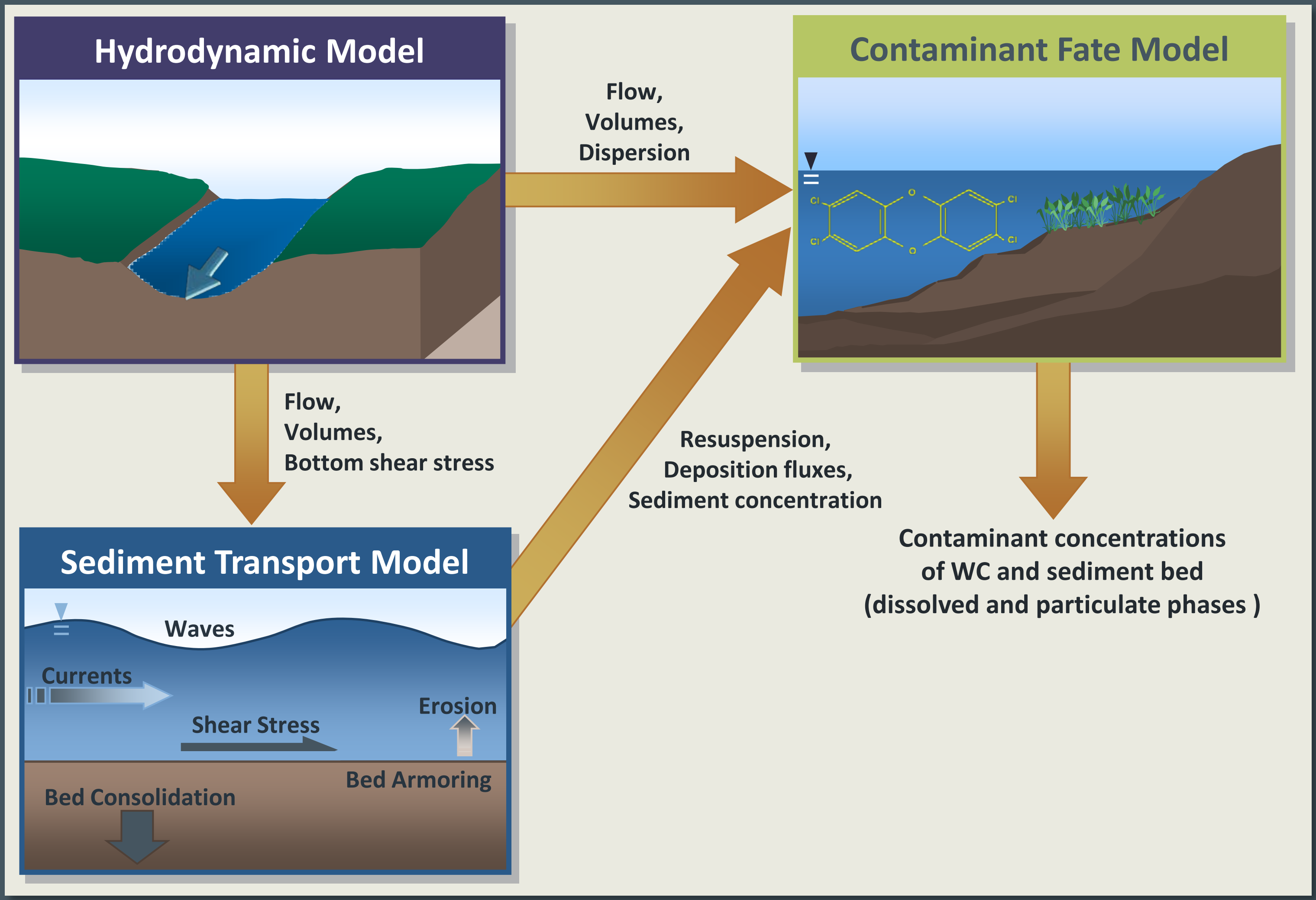
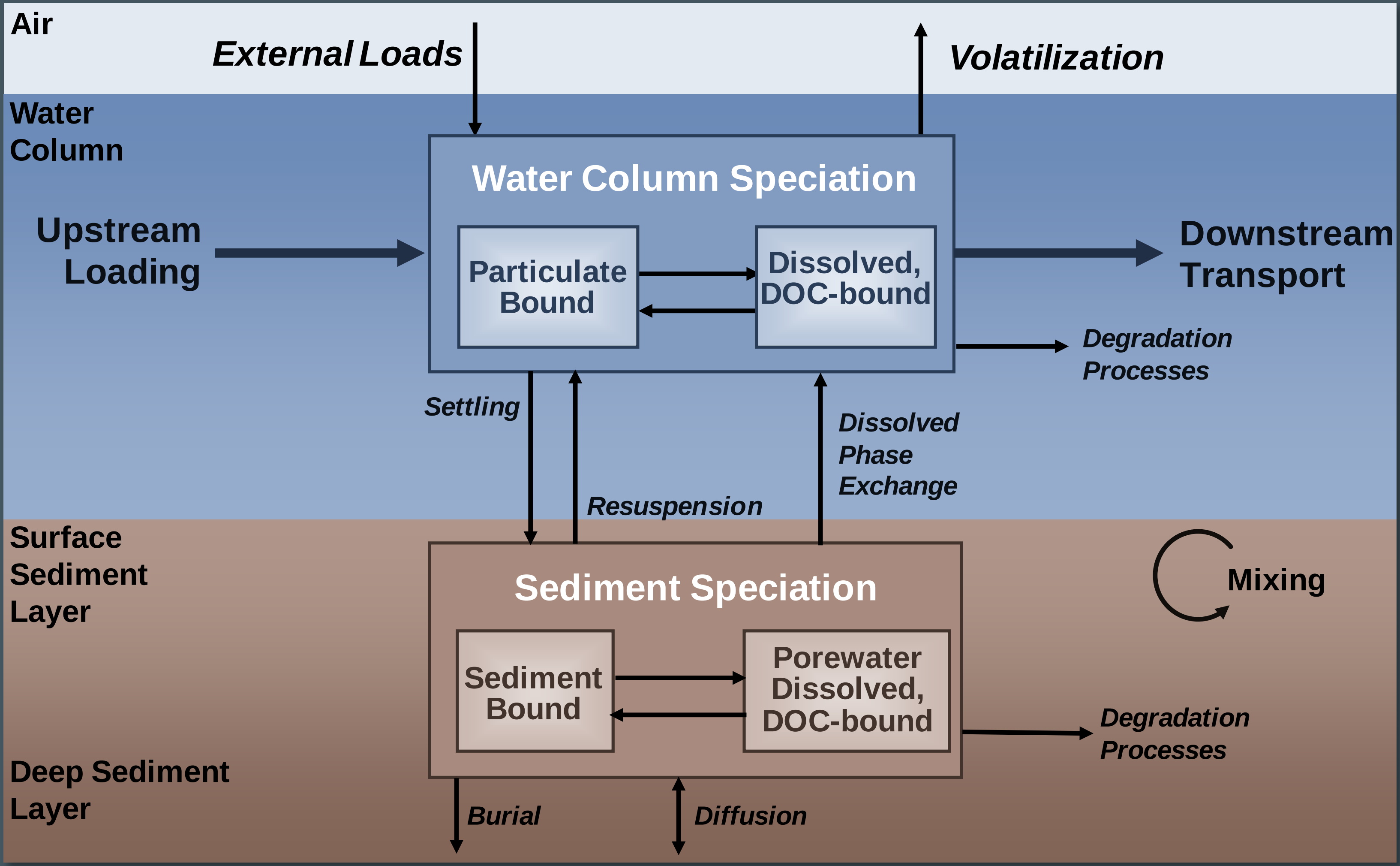
# Fate Model Structure and Processes

# Fate Model Linkages



# Processes Simulated by Fate Model



# Chemical Species Simulated by Model

- Calibration focused on 2378D and 2378F
  - Likely key risk drivers
- OCDD included as secondary focus
  - Provide means of differentiating regional sources from waste pit source
  - Adds robustness to calibration due to differing behavior (*Kow*) and spatial patterns

# Fate Model Development

# Fate Model Inputs – General

- Initial conditions
- Boundary conditions and loads
- Partitioning
- Fate and transport parameters
  - Organic carbon
  - Bed mixing and mass transfer
  - Volatilization



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# Fate Model Inputs – Summary

| Group | Input(s) | Data Source(s) | Approach |
|---|---|---|---|
| Initial Conditions | Starting D/F conc. in bed | 2002-2005 TMDL sediment data | Polygons mapped to model grid |
| Boundary Conditions | D/F conc. in water at:<br>• SJR Inflow<br>• HSC Inflow<br>• HSC Open | TMDL surface water data | Mean concentration from sample station(s) near boundary |
| External Loads* | Point sources<br>Runoff<br>Atmospheric deposition | TMDL sampling data | Apply loads calculated for TMDL model |
| Partitioning | $K_{OC}$<br>$K_{DOC}$ | TMDL water data; literature | 3-phase calculations from data; corroborated by literature |

**More detail provided on following slides*



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# Fate Model Inputs – Summary (cont.)

| Group | Input(s) | Data Source(s) | Approach |
|---|---|---|---|
| Organic carbon* | $f_{OC}$ in sediment | TMDL, RI sediment data | Correlation with grain size<br>Polygons mapped to model grid |
| | DOC in pore water | Literature | Constant value |
| | $f_{OC}$, DOC in water column | TMDL, long-term TCEQ water data | Average values from stations within model domain |
| Bed mass transport | Diffusion coefficients | Literature | Vary by chemical based on MW |
| | Porewater exchange coefficient | Literature/ calibration | Initial values based on experience at other sites; adjust during calibration |
| | Rate and depth of mixing (bioturbation) | | |
| Volatilization | Henry's Law constant | Literature | Vary by chemical |
| | Water temperature | NOAA gages | Annual cycle fitted through data |

**More detail provided on following slides*



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# Update: Expansion to Include OCDD

- Generally same approach used for TCDD/F inputs as described in Workshop #1
- Coordinating with University of Houston on external loads
  - OCDD concentrations measured, but loads not quantified for TMDL
  - OCDD loads will be calculated using TMDL methodology
    - Awaiting further information from University of Houston



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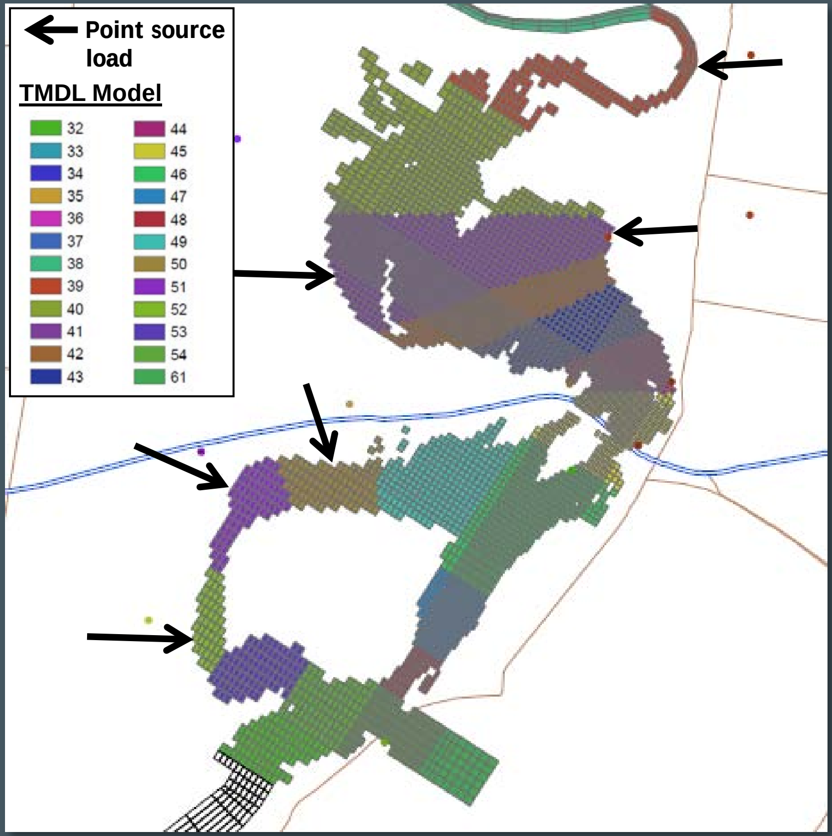
# Update: External Loads

- TCEQ Dioxin TMDL Study quantified external load estimation on an annual average basis
  - Point sources
    - Data gathered during Spring 2003 TMDL sampling
  - Stormwater runoff
    - Calculated based on land cover information, average congener concentrations in runoff samples, and rainfall
  - Direct (atmospheric) deposition
    - Calculated based on measured deposition fluxes and surface area of TMDL model segments
      - Average dry deposition flux for days with no rain
      - Average wet deposition flux for days with > 0.1” rainfall

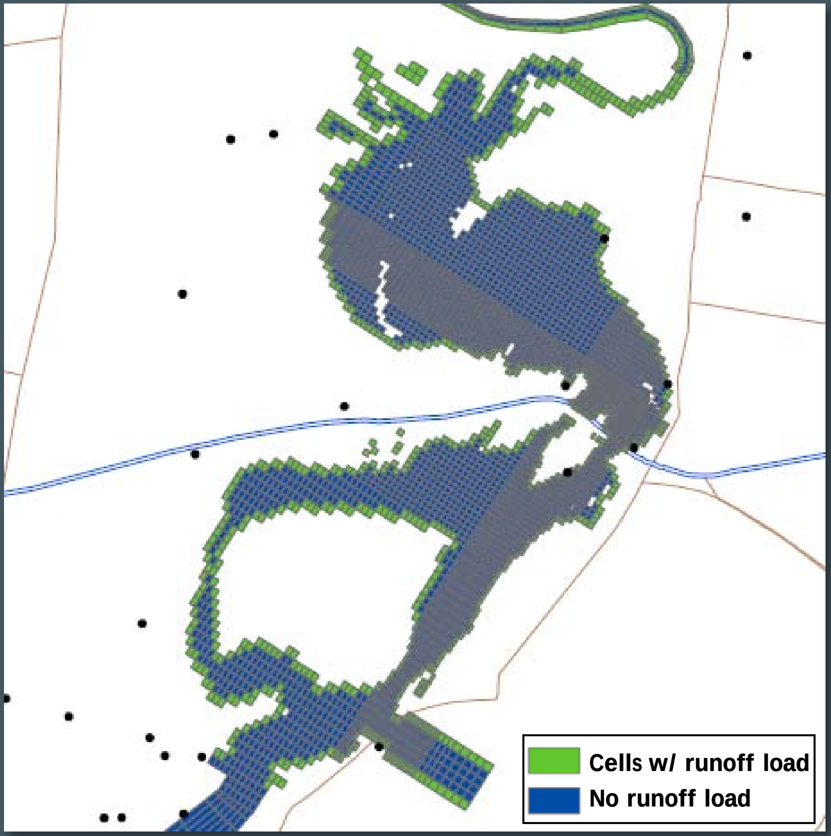
# External Loads

- TMDL loads mapped onto model grid

**Point, Atmospheric Loads**

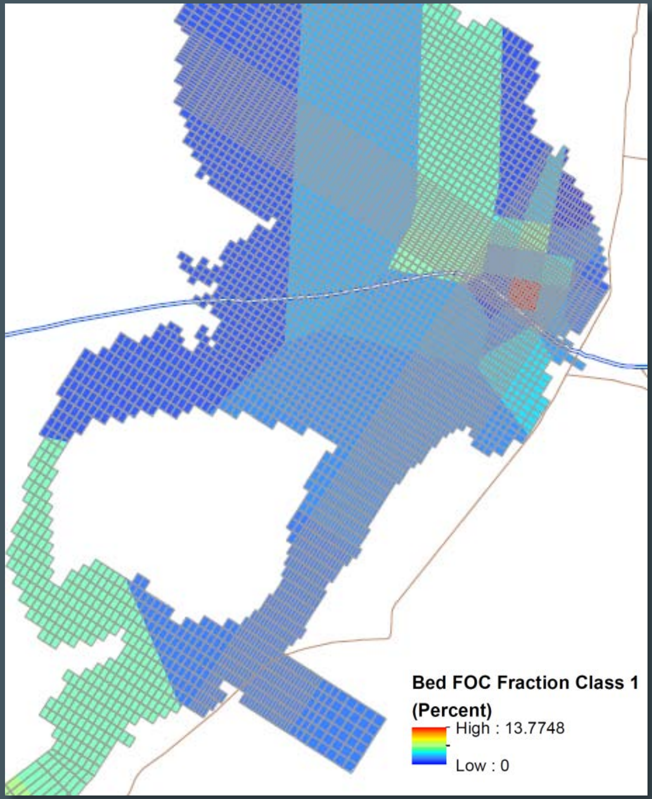



**Runoff Loads**



# Update:  Sediment Organic Carbon

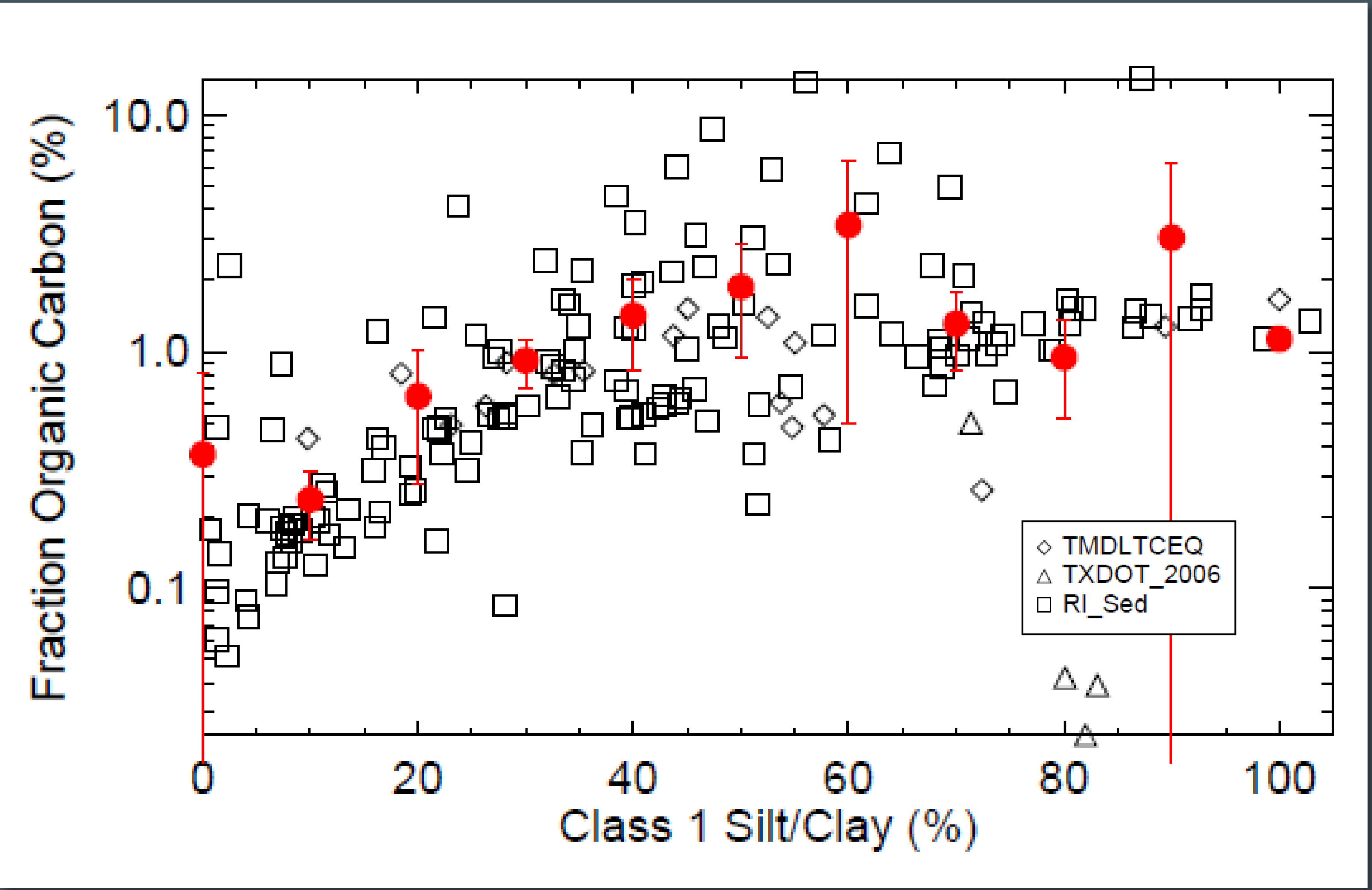
- Methodology
  - Generate Thiessen polygons of sediment $f_{oc}$ over study area (similar to initial conditions) to capture spatial variations in total carbon
  - At each polygon location, specify $f_{oc}$ of each size class such that
    - Total $f_{oc}$ is honored
    - Differences among size class $f_{oc}$ is honored



# Sediment Organic Carbon (cont.)

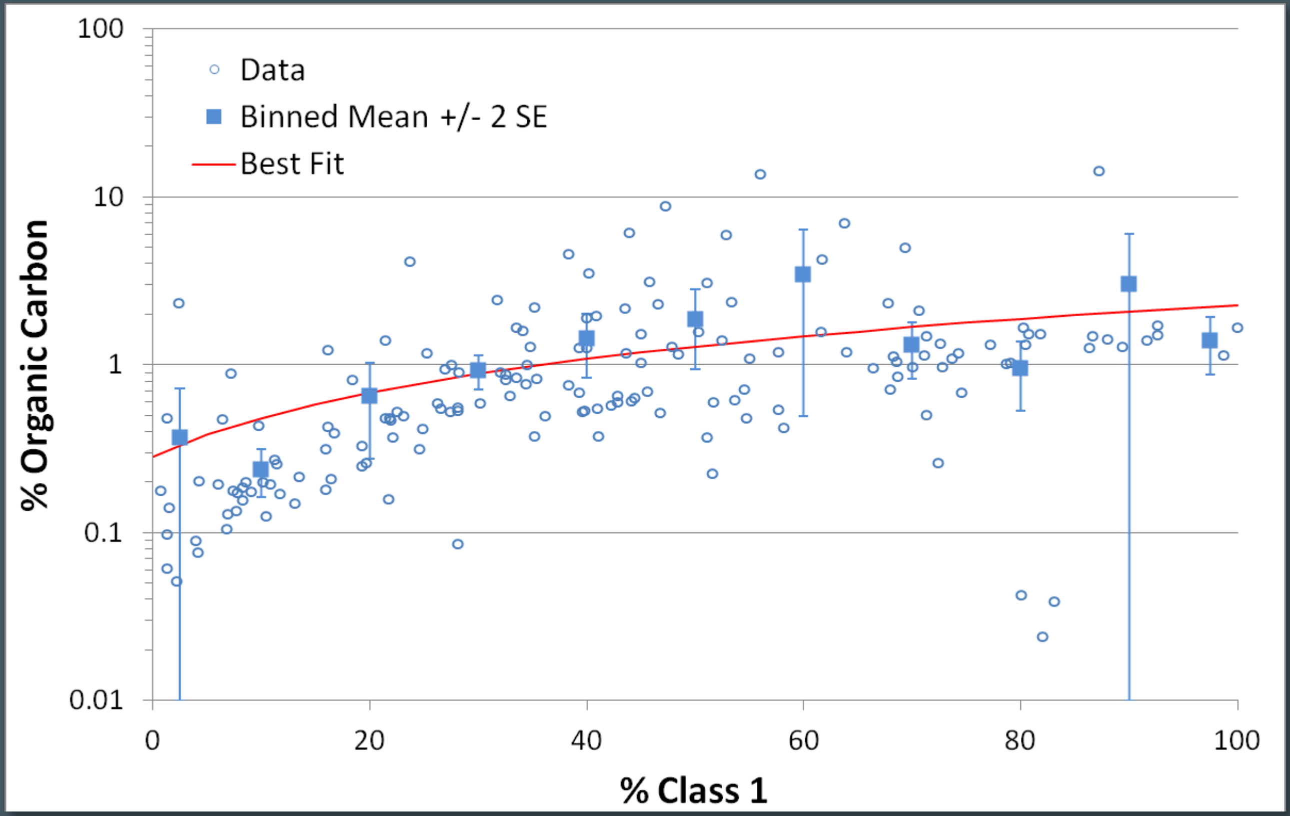
- Need to specify $f_{oc}$ for each of the four bed sediment size classes simulated by the sediment transport model
  - Class 1: <62 µm (silt/clay)
  - Class 2: 62–250 µm (fine sand)
  - Class 3: 250–2,000 µm (medium-coarse sand)
  - Class 4: >2,000 µm (gravel)
- Data suggest that $f_{oc}$ varies by size class

# Sediment Organic Carbon (cont.)



# Sediment Organic Carbon (cont.)

- "2 Class" model fit to identify relative difference in carbon content of Class 1 (silt/clay) vs. Class 2 - 4 (sand/gravel) sediments



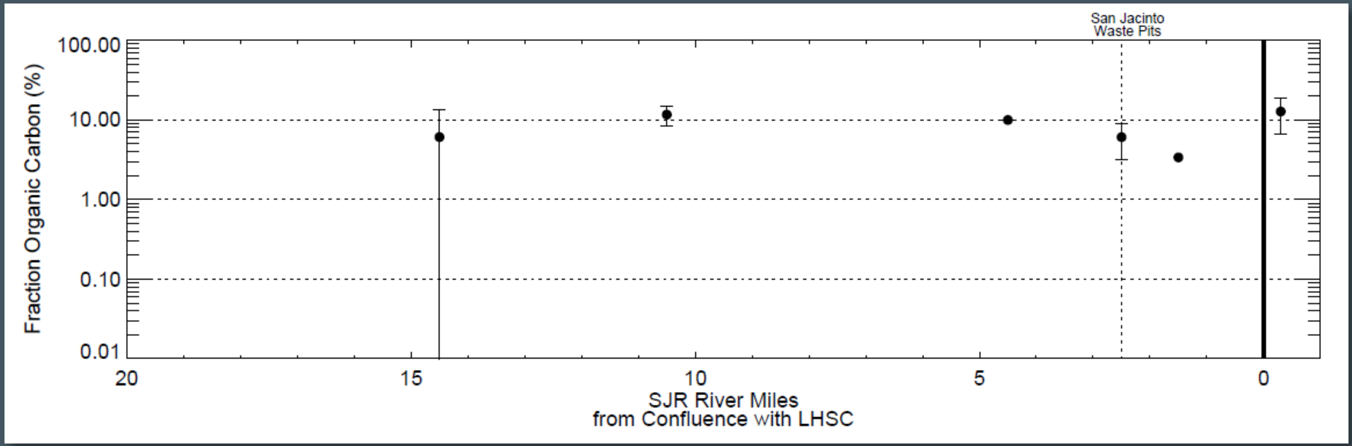
# Update: Water Column Organic Carbon

- Model requires fraction of organic carbon on particulate matter ($f_{oc}$) and DOC
- Two data sources used
  - TMDL data: limited number of sample events
    - Measured total and dissolved (TOC, DOC)
    - Particulate (POC) calculated by difference ($f_{oc}$ = POC/TSS)
  - Long-term TCEQ data
    - Routinely measure TOC and total/volatile suspended solids (TSS, VSS) at multiple locations within SJR
    - Estimated DOC and $f_{oc}$ two ways:
      1. Estimated DOC (and corresponding $f_{oc}$) based on observed TOC/DOC relationship in TMDL data set
      2. Estimated $f_{oc}$ from VSS/TSS

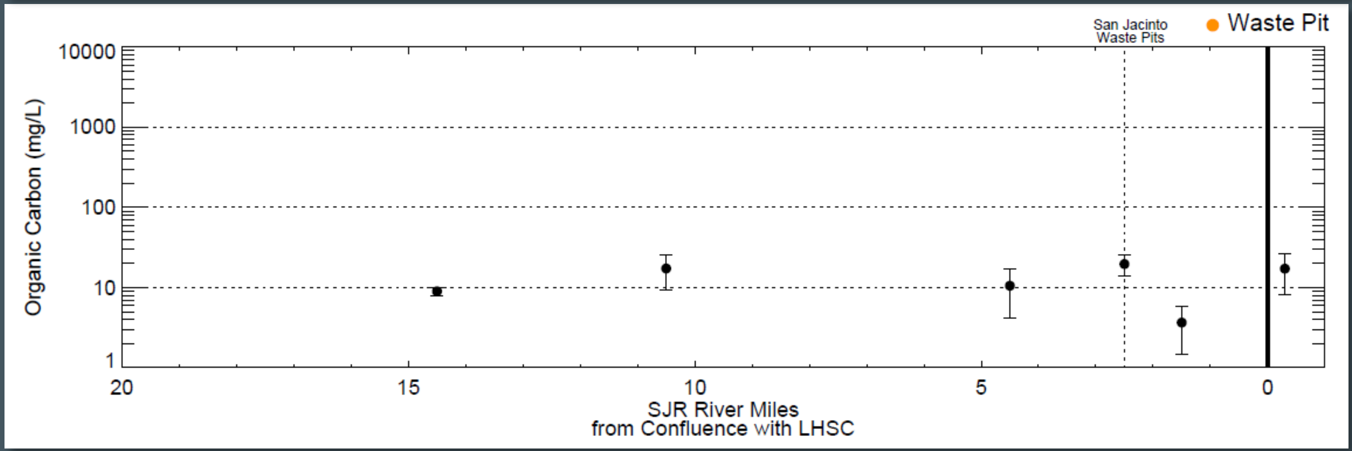
# Water Column Organic Carbon (cont.)

- TMDL dataset

$f_{oc}$



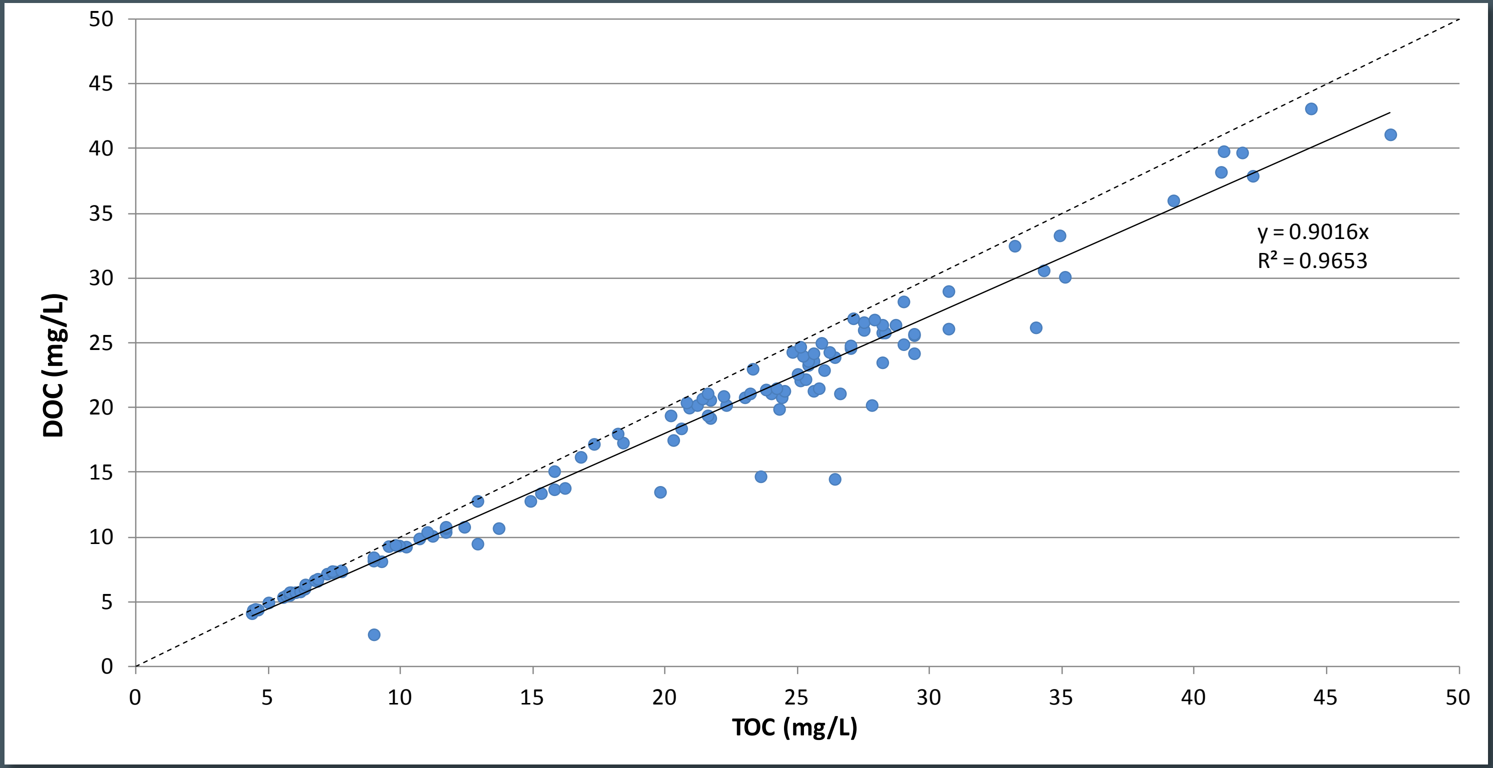

DOC




*** Outliers with calculated $f_{oc}$ greater than 40% removed**

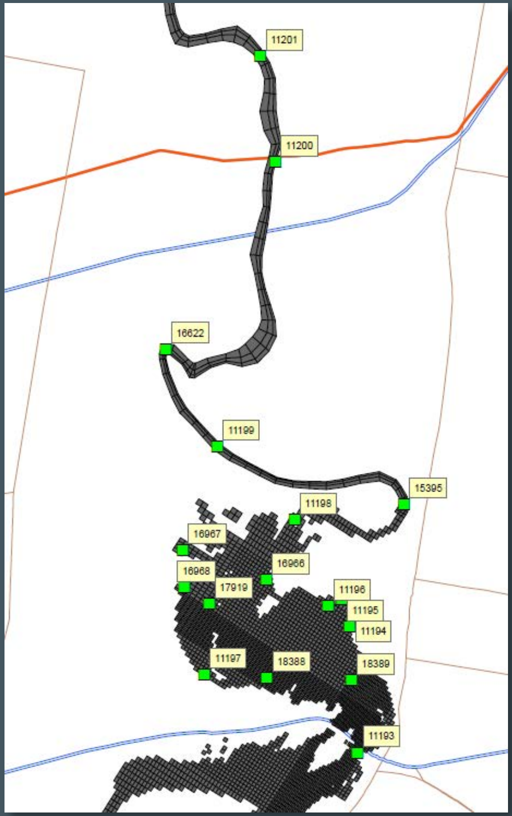
# Water Column Organic Carbon (cont.)

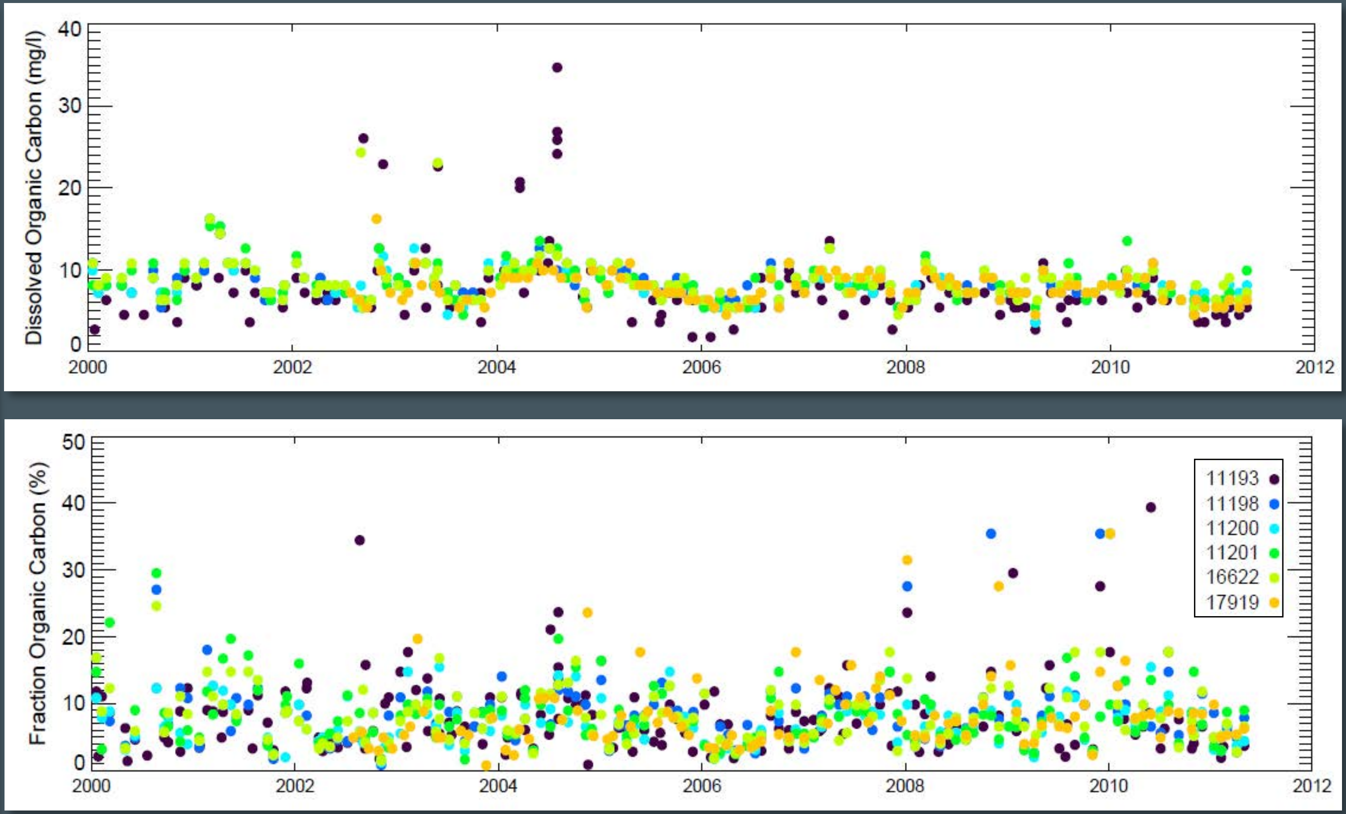
- TOC/DOC relationship in TMDL dataset



# Water Column Organic Carbon (cont.)

- Estimated DOC/ $f_{oc}$ for TCEQ dataset



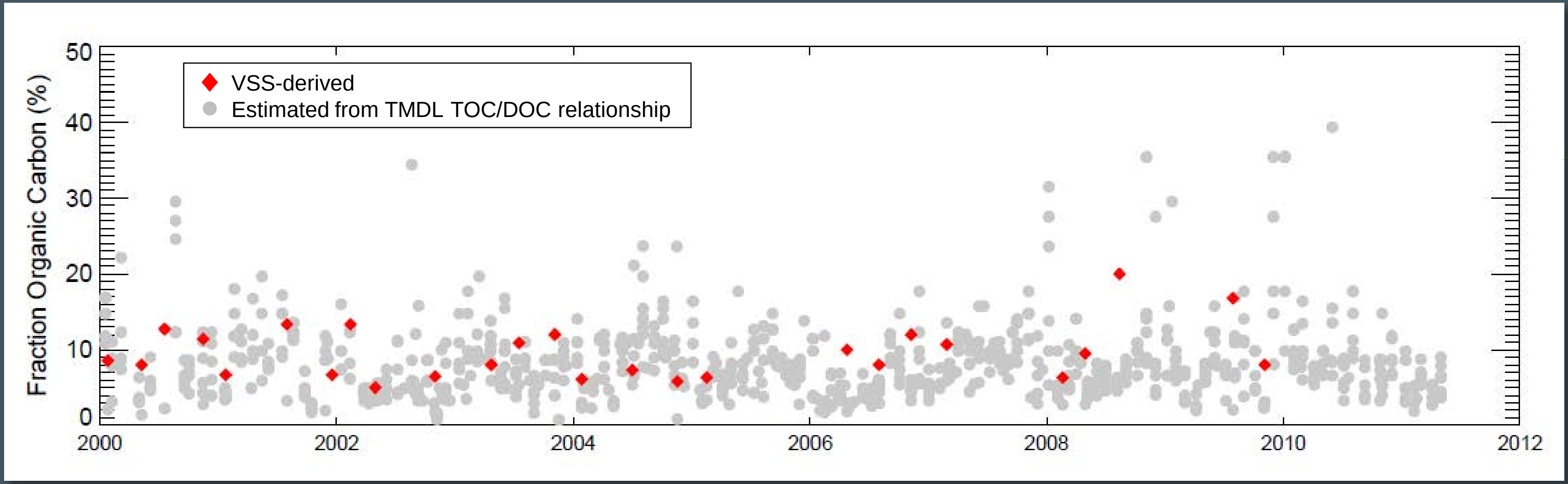




*Note: Legend indicates SJR station location IDs.*

# Water Column Organic Carbon (cont.)

- Estimated $f_{oc}$ from TCEQ TSS/VSS dataset

$$f_{oc} = \frac{VSS \times 0.4}{TSS}$$



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# Water Column Organic Carbon (cont.)

- Application in model
  - DOC
    - Spatially and temporally constant value of 10 mg/L
    - Combines TMDL and TCEQ datasets
  - $f_{oc}$
    - Spatially and temporally constant value of 9%
    - Combines TMDL and TCEQ data sets, including VSS-derived values
    - Similar to sediments, specify value for each sediment size class based on observed variation with grain size
      - Class 1: 9.9%
      - Classes 2-4: 1.2%

# Model Calibration Approach

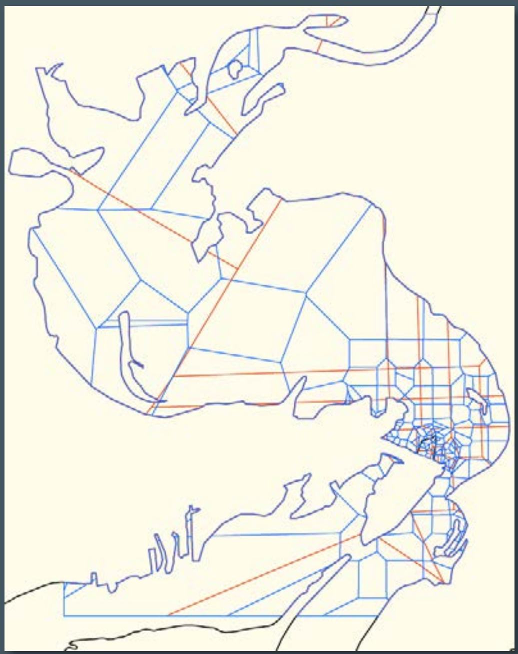
# Fate Model Calibration Approach

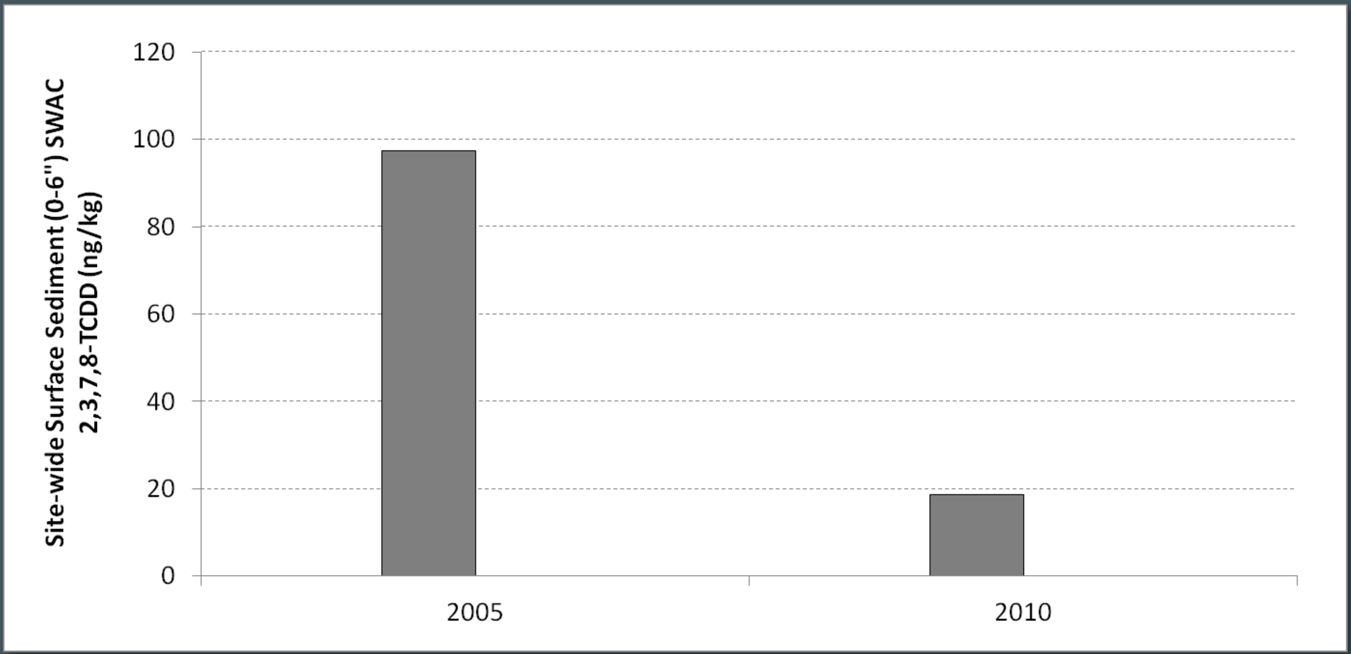
- Calibration period
  - Multi-year simulation (2005 to 2010) allows assessment of bed dynamics
  - Overlaps sediment transport calibration period
- Key calibration targets
  - **Sediment:** Approximately 5 times decline in area-weighted average 2378D/F concentration during calibration period
    - COPC Technical Memorandum (Integral and Anchor QEA 2011)
  - **Water column:** Spatial patterns from TMDL dataset
    - Changes in chemical speciation (total, dissolved, and particulate)
    - Differences among simulated chemicals (TCDD, TCDF, OCDD)

*Integral Consulting, Inc. and Anchor QEA, LLC, 2011. COPC Technical Memorandum - San Jacinto River Waste Pits Superfund Site, prepared for McGinnes Industrial Maintenance Corporation, International Paper Company, and U.S. Environmental Protection Agency, Region 6. May 2011.*

# Sediment Bed

- 2378D SWAC within site area

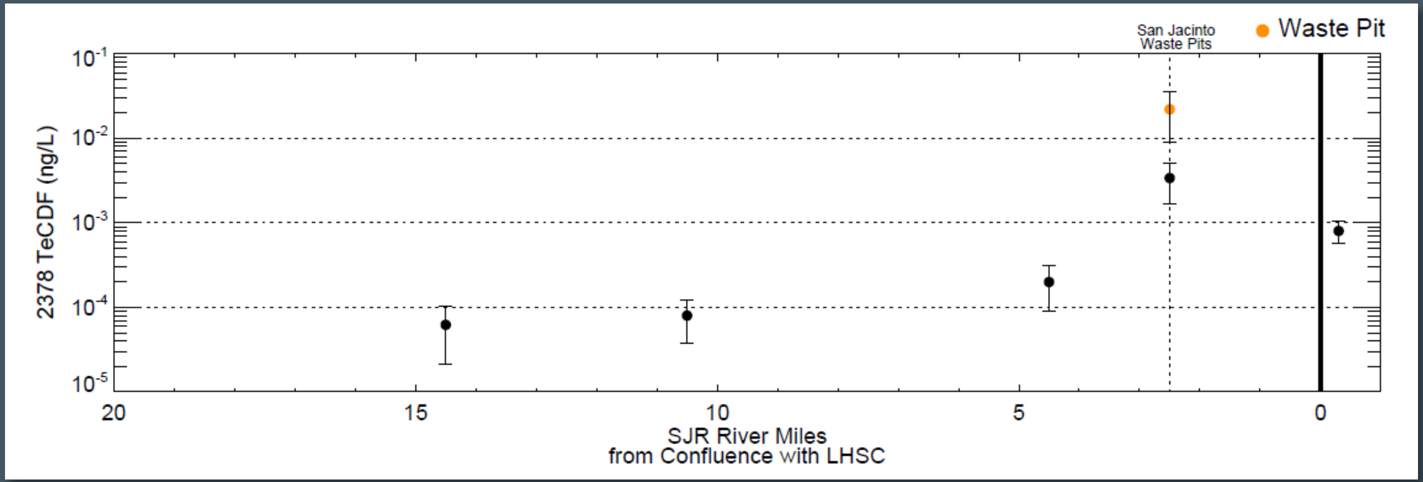




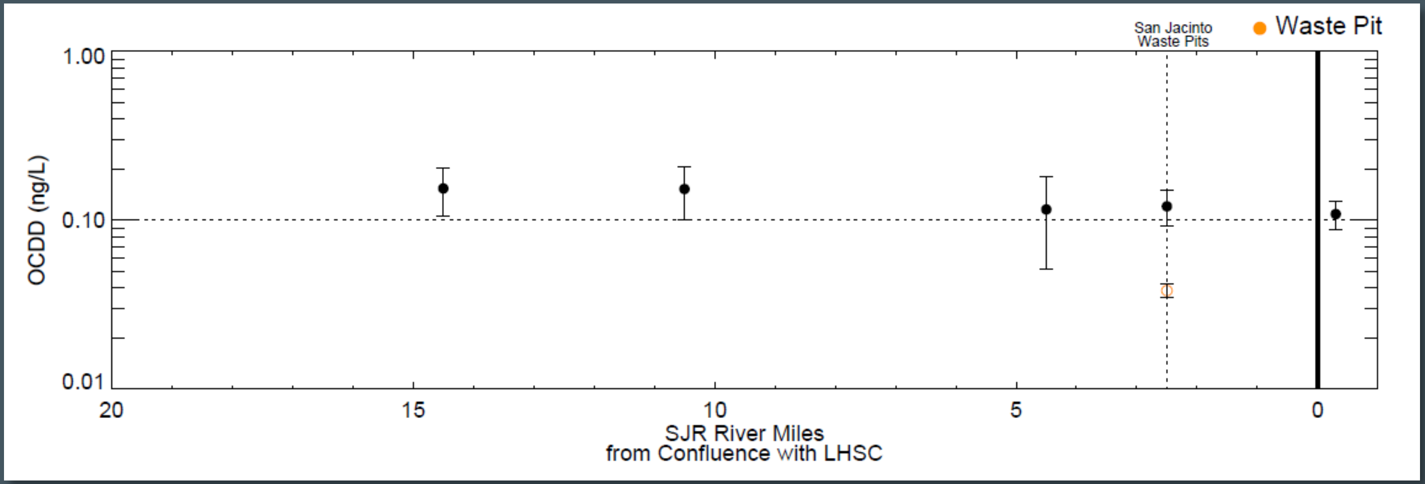

*Data-based SWACs from COPC Tech Memo (Integral and Anchor QEA, 2011).*

# Water Column Spatial Patterns

TCDF (Total)




OCDD (Total)




*Note: Open symbols represent averages where more than 50% of samples in the average are non-detect.*



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# Preliminary Model Calibration

- Initial contaminant fate model simulations completed for 6-year calibration period
  - Model is stable and mass balance closure is achieved
  - Run time: 26 hours
- Predicted water column results are in the general range of the data

# Model Calibration Approach

- Likely key calibration parameters
  - Sediment bed mixing rate and depth
  - Surface porewater exchange coefficient
- Sensitivity analysis
  - As part of calibration, key model parameters will be varied to evaluate model response and identify those to which the model is most sensitive
  - This will help understand key model uncertainties

# Status of Modeling

- Hydrodynamic model
  – Calibration complete
- Sediment transport model
  – Preliminary calibration complete
- Fate and transport model
  – Calibration initiated
- Modeling report scheduled for February 2012